N64-19985

CODE-1

NASA CR-53509

TECHNICAL REPORT NO. 349

GENERALIZED VISCOUS MULTICOMPONENT-

MULTIPHASE FLOW WITH APPLICATION TO

LAMINAR AND TURBULENT JETS OF HYDROGEN

By
Raymond Edelman
Harold Rosenbaum
Simon Slutsky

June 5, 1963

RESEARCH
ENGINEERING
PRODUCTION

AEROSPACE RESEARCH • AERODYNAMICS • PROPULSION • STRUCTURAL DYNAMICS • ELECTRONIC SYSTEMS AND INSTRUMENTS • COMPUTER MODULES

GENERAL APPLIED SCIENCE LABORATORIES, INC.

MERRICK and STEWART AVENUES, WESTBURY, L.I., N.Y. • (516) ED 3-6960

S9T-10166

TECHNICAL REPORT NO. 349

GENERALIZED VISCOUS MULTICOMPONENT-

MULTIPHASE FLOW WITH APPLICATION TO

LAMINAR AND TURBULENT JETS OF HYDROGEN

By
Raymond Edelman
Harold Rosenbaum
Simon Slutsky

Prepared for

George C. Marshall Space Flight Center
Huntsville, Alabama
Under Contract No. NAS.8-2686

Prepared by

General Applied Science Laboratories, Inc.
Merrick and Stewart Avenues
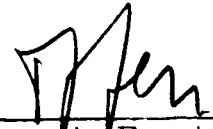Westbury, L.I., New York

June 5, 1963

Approved By _____
Antonio Ferri
President

TABLE OF CONTENTS

ABSTRACT

1 9985

A

A model is established for the continuum flow of a multicomponent system of gases and their condensed phases. The general conservation equations governing the behavior of the gases and condensed phases are derived. Viscosity, heat conductivity, diffusion and production of species by chemical reactions are included in the development. Non-equilibrium phenomena associated with the presence of condensed phases is discussed in some detail.

Preliminary application to the high altitude hydrogen dumping process is made in an analysis and numerical calculation on a chemically frozen (diffusion controlled) axisymmetric jet in phase equilibrium.

Arthur

LIST OF SYMBOLS

x	Streamwise coordinate
r	Radial coordinate
p	Pressure
R	Gas constant
T	Temperature
W	molecular Weight
ρ	Mass concentration in mixture
$\dot{\sigma}_v,\ \dot{\sigma}_\ell$	Unilateral evaporation and condensation rate, respectively
$\dot{W}_v^F = \dot{\sigma}_v - \dot{\sigma}_\ell$	Production of gas by evaporation
v	Velocity
h	Static enthalpy
H	Stagnation energy
u	Internal energy
L	heat of phase change
δ	density
$\underline{f}$	Force of interaction between gas and condensed phases.
$\dot{Q}$	Heat transfer interaction between gas and condensed phases.
N_p	Droplet number concentration
$\dot{W}_v^c$	Production of gas by chemical reaction

Y_{v_i} Mass concentration of the ith gaseous species in the gas phase

X_{p_i} Mass concentration of the ith condensed species in the condensed

β_i Mass concentration of ith species in the mixture

$\underline{j_{vi}}$ Diffusional mass flux defined by equation 12

μ Viscosity

$\underline{\pi}$ Stress tensor

k Thermal conductivity

$\underline{q}$ Heat flux by conduction

C_D Drag coefficient defined by Eq. 37a

λ Heat transfer coefficient defined by Eq. 40a

h_D Mass transfer coefficient

R_e Reynolds No. $\left(\dfrac{\rho v\ r}{\mu}\right)$

P_r Prandtl No. $\left(\dfrac{C_p\ \mu}{k}\right)$

L_e Lewis No. $\left(\dfrac{\rho\ D\ C_p}{k}\right)$

N_u Nusselt No. defined in eq.'s 50 and 52 for heat and mass transfer, respectively

D_{ii} Binary diffusion coefficient

A_i', ω_i Constants in Eq. 57

Ψ Stream function defined by Eq. 83

ξ Transformed x coordinate defined by Eq. 85

U Non-dimensionalized streamwise velocity component

Subscripts

e	Free Stream
j	Jet
i	i^{th} species
p	Particle
g	Gas mixture
v	component in the gas phase
m	Total mixture

GENERALIZED VISCOUS MULTICOMPONENT-

MULTIPHASE FLOW WITH APPLICATION TO

LAMINAR AND TURBULENT JETS OF HYDROGEN

By

Raymond Edelman
Harold Rosenbaum
Simon Slutzky

I. INTRODUCTION

The dumping of combustibles overboard from stages of boost vehicles creates several problems of potential importance. The combustion, surface heating, and induced pressure forces acting on the missile surface are possible consequences of the dumping process. The problem is quite complex owing to the combined effects of finite rate chemistry and jet boundary layer interaction with the external flow. Investigations involving gaseous combustibles under conditions simulating launch trajectories are developed and discussed in Ref. (1, 2, 3, 4).

Common to these investigations is that the various species were present in the gas phase only. However, when cryogenic hydrogen is the fuel under consideration, it becomes necessary to consider the possibility of two-phase flow. In fact, a typical state in the hydrogen fuel tank consists of saturated liquid hydrogen at approximately $20^{\circ}K$ ($p \cong 1$ atm). Thus, at high altitudes, say of the order of 200,000 feet, it is possible to expand the hydrogen into the solid-vapor region. Furthermore, if the expansion is nearly

isentropic from 40 to 80% of the hydrogen can be in the solid phase (where $T \approx 10^{\circ}K$) depending on whether vapor or liquid is bled from the tank. It is clear, therefore, that the subsequent mixing with the surrounding air can lead to condensation of the air. In general then, we can expect the flow field to be comprised of the components of air and hydrogen each occuring in two-phases.

The problem of accounting for the effects due to the presence of condensed species can be divided into two parts: (1) development of the conservation equations for the flow field and (2) determination of constitutive relations for the transfer of mass, momentum, and energy between the phases. The first part involves the description of the conservation of mass, momentum, and energy for the gas phase and the condensed phase systems. The second part involves the description of the dynamic and thermodynamic interactions between the gas and condensed phase systems. In general, the second part involves the description of velocity differences between the phases (dynamic non-equilibrium), temperature differences (thermal non-equilibrium), and mass transfer between the phases (non-equilibrium phase changes). This latter process comes under the heading of condensation-evaporation kinetics.

The purpose of the present report is to provide a model from which a system of governing equations may be deduced and to indicate constitutive relations which may be used to account for the interaction phenomena. Finally, the results of the analysis are applied to special cases which are of present interest.

The authors gratefully acknowledge the useful discussions with Dr. Vito Agosta of the Polytechnic Institute of Brooklyn and Mr. Andrew Pouring of Yale University as well as the numerical calculations carried out by Mr. David Soll and the IBM 709 program written by Mr. Jay Hoffman.

II. ANALYSIS

In establishing a model for the present complex flow system it becomes necessary to make certain assumptions. These assumptions are, in general, made in regard to the nature of the condensed phase system. The basic assumptions are discussed below.

(1) The condensed phase is in the form of a cloud of solid or liquid particles. This assumption is more of a statement of fact evidenced by launch experience and wind tunnel studies relating to condensation of various gases (5).

(2) droplet-droplet interaction is negligible. That is, the condensed phase is assumed to form a dilute suspension in the gas phase.

(3) the volume occupied by the condensed phase is negligible. This is merely a statement of the fact that the mass density of a condensed species is much greater than the mass density of its vapor.

(4) random motion of the particles of condensed phase is assumed negligible. That is, pressure, temperature and transport properties associated with random motion are considered negligible compared with those of the gas phase. The validity of this assumption rests on the condition that the particle size be larger than that of the molecules in the gas phase.

(5) thermal radiation is neglected. The low temperature with which we are concerned implies that thermal radiation will be negligible.

(6) each droplet has a uniform temperature at any instant. That is, conduction (and convection within the droplet in the case of liquid droplets) is negligible. In general, droplet sizes will be small enough to render this assumption valid.

(7) we shall assume that the state of the vapor at the droplet surface corresponds

to the droplet temperature and velocity. This assumption is made in order to

provide a means of systematically accounting for the condensed phase-gas phase

interactions.

(8) surface energy, gravity and electric charge effects an neglected.

In general, the approach will be to develop a system of governing

equations which will describe the behavior of the gas phase globally and the

condensed species individually. This permits the gases to be treated as a

multicomponent diffusing system with chemical reactions in the way previously

developed for gaseous systems (see e.g. Ref. 6). On the other hand, the

condensed species are treated individually so that the mass, momentum, and

thermal interactions can be handled in terms of the best available information

for flow about bodies under the conditions which can prevail in the present inves-

tigation. We refer to these relations as the constitutive relations. A discussion

of these relations will be taken up after the general conservations equations are

derived.

In accordance with assumption (7), each droplet may be thought to

have a film of vapor surrounding it. Within this film, velocity and temperature

are brought from the gas-phase values to the values at the droplet surface. Since

the film is vapor, it is associated with the gas phase but is considered to contain

negligible mass. This implies that the instantaneous flow of mass, momentum

and energy from theparticles is equal to the instantaneous gain of mass,

momentum and energy by the gas phase. Thus, the film is the source of irrever-

sible entropy production due to the non-equilibrium transfer of mass, momentum and

energy between the phases. It must be noted that the mass transfer which is due to evaporation and condensation has an associated momentum and energy transfer. These are in addition to the momentum and energy transfers due to velocity and temperature differences, respectively. Let us consider this point in more detail as follows. In the first place, assumption (2) implies that the influence of the condensed pahse on the flow field may be constructed in terms of the interactions associated with a single particle and its surroundings multiplied by a local number density of droplets in the elemental volume of mixture. This permits the use of available information for the interaction of single droplets in an infinite fluid. Further, the introduction of the local number density "smears" out the actual discrete nature of droplet system. The result of this is to predict a local, as well as overall, average effect of the droplets on the flow field. We consider first, the mass, momentum and energy transfers with the evaporation and condensation process.

Mass Transfer: The process of evaporation is composed of a simultaneous unilateral evaporation rate, $\dot{\sigma}_v$, and a unilateral condensation rate. The net result of the two unilateral rates is the evaporation rate. Thus, we have:

$$\dot{W}_v^F = \dot{\sigma}_v - \dot{\sigma}_\lambda$$

Clearly, if this difference is negative we have condensation and if it is zero there is, in effect, no phase change.

Momentum: The droplet loses momentum at a rate equal to $\dot{\sigma}_v \underline{V}_p$ and simultaneously gains momentum at a rate equal to $\dot{\sigma}_l \underline{V}_p$. This is in accordance with the condition that at the interface the vapor and droplet have the same velocity $\underline{V}_p$. Thus, the net loss of droplet momentum is given by:

$$\underline{V}_p \left(\dot{\sigma}_v - \dot{\sigma}_\lambda \right) = \underline{V}_p \dot{W}_v^F \qquad 2$$

This represents a gain in gas phase momentum due to evaporation.

Energy: The droplet energy loss associated with the unilateral evaporation rate is composed of condensed phase enthalpy, kinetic energy, and the heat of vaporization. The gain of droplet energy associated with the unilateral condensation rate is composed of the vapor enthalpy and kinetic energy evaluated at the interface state. Thus, the net loss of droplet energy is given by:

$$\dot{\sigma}_v \left(h_p + L + \frac{\underline{V}_p \cdot \underline{V}_p}{2} \right) - \dot{\sigma}_\lambda \left(h_{v_{T_p}} + \frac{\underline{V}_p \cdot \underline{V}_p}{2} \right) =$$

$$= \dot{W}_v^F \left(h_p + L + \frac{\underline{V}_p \cdot \underline{V}_p}{2} \right) \qquad 3$$

Note that the droplet gives up the heat of vaporization and gains the heat of condensation where:

$$h_{v_{T_p}} = h_p + L \qquad 4$$

In addition, the interface moves in accordance with the rate of evaporation of the droplet. This results in a work transfer given by:

$$P_p / \sigma_\lambda \, \dot{W}_v^F \qquad 5$$

where,

$$P_p \equiv \text{interface pressure}$$

$$\delta_l \equiv \text{droplet density}$$

$$\frac{\dot{W}_v^F}{\delta_l} \equiv \text{rate of increase in gas phase volume due to droplet}$$

evaporation

Since, in general, $L \gg P_p/\delta_1$, the energy associated with **Eq. 5** is negligible

compared with that given by **Eq. 3**.

It has been pointed out that in addition to mass, momentum, and

energy transfers associated with evaporation, there exist dynamic and thermal

interactions in virtue of the velocity and temperature non-equilibrium between

the phases, respectively. These are discussed, in order, in the following.

Drag Force :

The drag force constitutes a momentum interchange between the

phases. We shall assume that this force is purely a viscous phenomenon and

depends only on the velocity difference, i. e.:

$$\underline{f_p} = \underline{f_1}(\underline{v_v} - \underline{v_p}) \tag{6}$$

Additional forces exist but can be shown to be, in general, of higher order (Ref. 7).

Thermal Interaction:

This thermal interaction which is dependent on the temperature

difference between the phases is merely a statement of convective heat transfer.

This precludes the existence of radiation heat transfer in accordance with assumption (5). This convective heat transfer is expressed by:

$$\dot{Q}_P = \dot{Q}_P(T_v - T_P) \qquad 7$$

In constructing the conservation equations, we shall consider the existence of chemical reactions and assume that these take place in the gas phase.

Conservation Equations:

In consideration of the above discussion, we are now in position to write down the conservation equations in a systematic manner.

In order to maintain generality, we consider i gaseous species and i condensed species i.e. each component can exist in each phase. We consider each condensed species individually. The implication of this treatment of the condensed phase is discussed in a later section dealing with phase equilibrium of multicomponent systems but does not influence the following development.

Continuity of Mass:

For the ith gaseous species:

$$\nabla \cdot \rho_{vi} \underline{V}_{vi} = \dot{W}_{vi}^r + \dot{W}_{vi}^c \qquad 8$$

Where,

$$\sum_i \dot{W}_{vi}^c = 0$$

$$\sum_i \dot{W}_{vi}^F \qquad = \text{Net production of gas phase mass due to evaporation}$$

$$\sum_i \left(\dot{W}_{vi}^r + \dot{W}_{pi}^r \right) = 0$$

For the ith <u>condensed species:</u>

$$\nabla \cdot \rho_{pi} \underline{V}_{pi} = \dot{W}_{pi}^{F} = -\dot{W}_{vi}^{F}$$

9

In order that the species in the gaseous phase may be treated in the usual manner we introduce the following barycentric (mass mean) quantities:

$$\rho_g = \sum_i \rho_{vi}$$

10

$$\rho_g \underline{V}_g = \sum_i \rho_{vi} \underline{V}_{vi}$$

11

and

$$\underline{j}_{vi} = \rho_{vi} \left(\underline{V}_{vi} - \underline{V}_g \right)$$

12

where we further introduce the gas phase mass fractions given by:

$$Y_{vi} = \frac{\rho_{vi}}{\rho_g}$$

13

where,

$$\sum_i Y_{vi} = 1$$

14

Introducing the definitions 10 - 13 into Eq. 8 gives:

$$\nabla \cdot \rho_g \underline{V}_g Y_{vi} = \dot{W}_{vi}^{F} + \dot{W}_{vi}^{c} - \nabla \cdot \underline{j}_{vi}$$

15

which is the "species conservation" equation for the ith gaseous species. If Eq. 15 is summed over all i gaseous species, noting Eq. 14, we get the "global continuity" equation for the gaseous system:

$$\nabla \cdot \rho_g \underline{V_g} = \sum_i \dot{W}_{vi}^F \qquad 16$$

In applying the present analysis it will be convenient to introduce a variable for the condensed phase mass fractions defined by:

$$X_{pi} = \frac{\rho_{pi}}{\rho_p} \qquad 17$$

where

$$\rho_p = \sum_i \rho_{pi} \qquad 18$$

and

$$\sum_i X_{pi} = 1 \qquad 19$$

Thus, Eq. 9 for the continuity of mass for the ith species of the condensed phase:

$$\nabla \cdot \rho_p V_{pi} X_{pi} = \dot{W}_{pi}^F \qquad 20$$

Momentum:

The global gas-phase momentum equation may be written:

$$\nabla \cdot \sum_i \rho_{v_i} \underline{V}_{v_i} \underline{V}_{v_i} = \nabla \cdot \underline{\Pi}_g + \sum_i \underline{f}_{(\sum_j \rho_j)v_i} + \sum_i \dot{W}_{v_i}^F \underline{V}_{\rho_i} \qquad 21$$

where the summation notation, $\sum_i \underline{f}_{(\sum_j \rho_j)v_i}$, reads, "the force of all

j particles acting on the ith gas species summed over all i gas species". In

terms of the barycentric quantities Eq. 21 with the aid of Eq. 16 becomes:

$$\rho_g \underline{V}_g \cdot \nabla \underline{V}_g = \nabla \cdot \underline{\Pi}_g + \sum_i \underline{f}_{(\sum_j \rho_j)v_i} + \sum_i \dot{W}_{v_i}^F (\underline{V}_{\rho_i} - \underline{V}_g) \qquad 22$$

The ith condensed-phase momentum equation is given by:

$$\nabla \cdot \rho_{\rho_i} \underline{V}_{\rho_i} \underline{V}_{\rho_i} = \underline{f}_{(\sum_j v_j)\rho_i} + \dot{W}_{\rho_i}^F \underline{V}_{\rho_i} \qquad 23$$

which with the aid of Eq. 19 may be written:

$$\rho_{\rho_i} \underline{V}_{\rho_i} \cdot \nabla \underline{V}_{\rho_i} = \underline{f}_{(\sum_j v_j)\rho_i} \qquad 24$$

Energy:

The combined gas-phase energy equation in terms of the barycentric

quantities is given by:

$$\nabla \cdot \rho_g \left(u_g + \frac{\underline{v}_g \cdot \underline{v}_g}{2}\right)\underline{v}_g = -\nabla \cdot \underline{q}_g + \nabla \cdot \underline{\pi}_g \cdot \underline{v}_g - \sum_i \nabla \cdot \underline{j}_{v_i} h_{v_i}$$

$$+ \sum_i \dot{Q}_{(E_\beta)v_i} + \sum_i \sum_j \underline{f}_{p_j v_i} \cdot \underline{v}_{p_i}$$

$$+ \sum_i \dot{W}_{v_i}^F \left(h_{p_i} + L_i + \frac{\underline{v}_{p_i} \cdot \underline{v}_{p_i}}{2}\right) \qquad 25$$

the ith condensed-phase energy equation is given by:

$$\nabla \cdot \rho_{p_i}\left(u_{p_i} + \frac{\underline{v}_{p_i} \cdot \underline{v}_{p_i}}{2}\right)\underline{v}_{p_i} = \underline{f}_{(\sum_j v_j)p_i} \cdot \underline{v}_{p_i} + \dot{Q}_{(\sum_j v_j)p_i}$$

$$- \dot{W}_{v_i}^F \left(h_{p_i} + L_i + \frac{\underline{v}_{p_i} \cdot \underline{v}_{p_i}}{2}\right) \qquad 26$$

SUMMARY OF CONSERVATION EQUATIONS:

The equations developed, as initially proposed, govern the mean mass flow field of the gas-phase and the individual flow behavior of the condensed-phase. It is also of interest to consider the "mixture" equations as a possible set of working relations. These equations are obtained by merely summing over all species in all phases. The resulting equations are listed below.

Continuity of Mass:

Mixture:

$$\nabla \cdot \left(\rho_g \underline{v}_g + \sum_i \rho_{p_i} \underline{v}_{p_i}\right) = 0 \qquad 27$$

ith condensed phase:

$$\nabla \cdot \rho_{p_i} \underline{v}_{p_i} = \nabla \rho_p \underline{v}_{p_i} X_{p_i} = \dot{W}_{p_i}^F = -\dot{W}_{v_i}^F \qquad 28$$

ith gas phase:

$$\nabla \cdot \rho_g \underline{v}_g Y_{v_i} = \dot{W}_{v_i}^F + \dot{W}_{v_i}^C - \nabla \cdot \underline{j}_{v_i} \qquad 29$$

Momentum

Mixture:

$$\nabla \cdot \left(\rho_g \underline{V}_g \underline{V}_g + \sum_i \rho_{p_i} \underline{V}_{p_i} \underline{V}_{p_i} \right) = \nabla \cdot \underline{\underline{\Pi}}_g \tag{30a}$$

or,

$$\rho_g \underline{V}_g \cdot \nabla \underline{V}_g + \sum_i \rho_{p_i} \underline{V}_{p_i} \cdot \nabla \underline{V}_{p_i} = \nabla \cdot \underline{\underline{\Pi}}_g + \sum_i \dot{W}_{v_i}^r (\underline{V}_{p_i} - \underline{V}_g) \tag{30b}$$

ith condensed phase:

$$\rho_{p_i} \underline{V}_{p_i} \cdot \nabla \underline{V}_{p_i} = \underline{f}_{(\sum_j V_j) p_i} \tag{31}$$

Energy

Mixture:

$$\nabla \cdot \left[\rho_g \left(h_g + \frac{\underline{V}_g \cdot \underline{V}_g}{2} \right) \underline{V}_g + \sum_i \rho_{p_i} \left(h_{p_i} + \frac{\underline{V}_{p_i} \cdot \underline{V}_{p_i}}{2} \right) \underline{V}_{p_i} \right] = $$

$$= -\nabla \cdot \underline{q}_g + \nabla \cdot (\underline{\underline{\tau}}_g \cdot \underline{V}_g) - \sum_i \nabla \cdot \underline{j}_{v_i} h_{v_i} \tag{32a}$$

or

$$\rho_g \underline{V}_g \cdot \nabla \left(h_g + \frac{\underline{V}_g \cdot \underline{V}_g}{2} \right) + \sum_i \rho_{p_i} \underline{V}_{p_i} \cdot \nabla \left(h_{p_i} + \frac{\underline{V}_{p_i} \cdot \underline{V}_{p_i}}{2} \right)$$

$$= -\nabla \cdot \underline{q}_g + \nabla \cdot (\underline{\underline{\tau}}_g \cdot \underline{V}_g) - \sum_i \nabla \cdot \underline{j}_{v_i} h_{v_i} +$$

$$+ \sum_i \dot{W}_{v_i}^r \left[\left(h_{p_i} + \frac{\underline{V}_{p_i} \cdot \underline{V}_{p_i}}{2} \right) - \left(h_g + \frac{\underline{V}_g \cdot \underline{V}_g}{2} \right) \right] \tag{32b}$$

ith condensed phase:

$$\rho_{p_i} \underline{V}_{p_i} \cdot \nabla h_{p_i} = \dot{Q}_{(\sum_j V_j) p_i} - \dot{W}_{v_i}^F L_i \tag{33}$$

The above relations, 27, 28, 29, 30a or b, 31, 32a or b and 33 constitute

seven, 7, partial differential equations for the nine, 9, unknowns:

$$\rho_g \qquad \rho_{p_i}$$
$$\underline{V_g} \qquad \underline{V_{p_i}}$$
$$Y_{v_i} \qquad h_{p_i}$$
$$h_g$$
$$P_g$$
$$h_{v_i}$$

The additional relations are supplied by Eq.'s of state:

$$P_g = P_g(\rho_g, T_g, Y_{v_i}) \qquad\qquad 34$$

$$h_g = \sum_i Y_{v_i} h_{v_i}(T_g) \qquad\qquad 35$$

$$u_{p_i} \cong h_{p_i}(T_{p_i}) \qquad\qquad 36$$

We note that this discussion assumes knowledge of the dependence of q_g, τ_g and j_{v_i} on the above variables. The discussion of these relations is taken up in the next section where similar relations for gas-phase condensed phase interactions are discussed.

III. CONSTITUTIVE RELATIONS FOR THE RATE PHENOMENA

In order to complete the necessary set of governing equations we must supply relations for $\underline{f}_i$, $\dot{Q}_i$, $\dot{W}_{v_i}$, $\underline{q}_g$, τ_g, and j_{v_i}. There exists no available theory for the description of the above six rate parameters occuring simultaneously. The kinetics of condensation and evaporation itself is not fully understood and forms the basis for many current investigations (Ref. 8). The problem of nucleation, condensation and evaporation, from both molecular and macroscopic approaches is reviewed extensively in Ref. 5. On the basis of available information it has been suggested that a semi-empirical approach would be the most fruitful direction to adopt in the present complex problem.[*]

Drag Force (f_{P_i}) We have indicated (see Eq. 6) that the drag force on a particle depends on the velocity difference. In terms of a drag coefficient, C_{D_i} , the force on a single droplet in the condensed phase is given by:

$$\frac{f_{(\sum_j V_j) P_i}}{N_{P_i}} = \frac{f_{g P_i}}{N_{P_i}} = \frac{f_{P_i}}{N_{P_i}} = \frac{C_{D_i} \bar{A}_i \rho_g}{2} \left(V_g - V_{P_i} \right) \left| V_g - V_{P_i} \right| \tag{37a}$$

This discription assumes that all particles associated with the local number concentration, N_{P_i} , have the same average size. This restriction may be removed by introducing an appropriate size distribution law (Ref. 9). A $C_D \bar{A}$ would then be determined for each size group within the local number concentration. Equation 37a may be rewritten to provide the total force per unit volume of mixture and is given by:

$$f_{P_i} = \frac{\rho_{P_i}}{m_{P_i}} C_{D_i} \bar{A}_i \frac{\rho_g}{2} \left(V_g - V_{P_i} \right) \left| V_g - V_{P_i} \right| \tag{37b}$$

In application, we shall assume that the droplets are spherical in shape so that Eq. 37b may be written:

$$f_{P_i} = \frac{3}{8} \rho_{P_i} \frac{C_{D_i} \rho_g}{\delta_{l_i} r_{P_i}} \left(V_g - V_{P_i} \right) \left| V_g - V_{P_i} \right| \tag{37c}$$

If the flow is in the Stokes regime then:

$$C_{D_i} = \frac{24}{Re_i} = \frac{12 \mu_g}{\rho_g r_{P_i} \left| V_g - V_{P_i} \right|} \tag{38}$$

and we get:

$$f_{p_i} = \frac{9}{2} \frac{\rho_{p_i} \mu_g}{\delta_i \, r_{p_i}^2} (v_g - v_{p_i})$$
<div align="right">39</div>

Thus, Eq. 39 or, in general, Eq. 37c may be used to account for the drag force between the gas phase and condensed phase.

Heat Transfer($\dot{Q}_{p_i}$) : The heat transfer between the gas phase and condensed phase depends on the temperature difference and can be expressed in terms of Newton's Law of Cooling. In terms a heat transfer coefficient, this is given by:

$$\frac{\dot{Q}_{(\Sigma \, v_j) p_i}}{N_{p_i}} = \frac{\dot{Q}_{p_i}}{N_{p_i}} = h \, A_i (T_g - T_{p_i})$$
<div align="right">40a</div>

Thus, the heat transfered per unit volume of mixture to the ith condensed species is given by:

$$\dot{Q}_{p_i} = \frac{\rho_{p_i}}{m_{p_i}} h_i A_i (T_g - T_{p_i})$$
<div align="right">40b</div>

and for spherical particles we get:

$$\dot{Q}_{p_i} = \frac{3 \rho_{p_i} h_i}{\delta_i \, r_{p_i}} (T_g - T_{p_i})$$
<div align="right">40c</div>

The coefficient λ_i is dependent on the rate of evaporation, $\dot{W}_{v_i}$, in virtue of the fact that this diffusing vapor is heated in flowing away from the droplet. The following development for λ_i is based on the work in Ref's 10 and 11.

We assume that the heat and mass transfer from the droplet is a quasi-steady process. The conduction term is modified by a correction factor, C_H, to account for convective heat transfer. Thus, the heat transfered to a single droplet in the ith condensed phase is given by:

$$\frac{\dot{Q}_{p_i}}{N_{p_i}} = 4\pi r^2 k_i C_{H_i} \frac{dT}{dr} - \left(\dot{W}_{v_i}^F\right)_p C_{p_i} (T - T_{p_i}) \qquad 41$$

In virtue of the quasi-steady assumption, Eq. 41 may be integrated from $r = r_p$ to $r = \infty$ to give:

$$\frac{\dot{Q}_{p_i}}{N_{p_i}} = 4\pi k_i C_{H_i} r_{p_i} (T_g - T_{p_i}) \left\{ \frac{\frac{\left(\dot{W}_{v_i}^F\right)_p C_{p_i}}{r_{p_i} 4\pi k_i C_{H_i}}}{e^{\frac{\left(\dot{W}_{v_i}^F\right)_p C_{p_i}}{r_{p_i} 4\pi k_i C_{H_i}}} - 1} \right\} \qquad 42$$

Now, we note that as $\dot{W}_{v_i} \to 0$ the term in the brackets approaches unity, i.e.

$$\lim_{\dot{W}_{v_i}^F \to 0} \left\{ \quad \right\} \to 1 \qquad 43$$

and we get:

$$\frac{\dot{Q}_{p_i}}{N_{p_i}} = 4\pi k_i C_{H_i} r_{p_i} (T_g - T_{p_i}) \qquad 44$$

The usual definition of the film coefficient is given by:

$$\frac{\dot{Q}_{P_i}}{N_{P_i}} = h_{H_i}\, 4\pi\, r_{P_i}^2\, (T_g - T_{P_i})$$

45

so that by comparison we get:

$$C_H = \frac{h_{H_i}\, r_{P_i}}{k_i} = \frac{1}{2}(N_u)_H$$

46

Therefore, returning to Eq. 42, we may write:

$$\frac{\dot{Q}_{P_i}}{N_{P_i}} = 4\pi\, r_{P_i}^2\, h_{H_i}\, (T_g - T_{P_i}) \left\{ \frac{\dfrac{(\dot{W}_{v_i}^F)_p\, C_{P_i}}{4\pi\, r_{P_i}^2\, h_{H_i}}}{e^{\frac{(\dot{W}_{v_i})_p C_{P_i}}{4\pi r_{P_i}^2 h_{H_i}}} - 1} \right\}$$

47

or,

$$\dot{Q}_{P_i} = \frac{3\rho_{P_i}}{\delta\lambda_i\, r_{P_i}}\, h_{H_i}\, (T_g - T_{P_i}) \left\{ \right\}$$

48

so that by Eq. 40c, we have:

$$\lambda_i = h_{H_i} \left\{ \frac{\dfrac{(\dot{W}_{v_i}^F)_p\, C_{P_i}}{4\pi\, r_{P_i}^2\, h_{H_i}}}{e^{\frac{(\dot{W}_{v_i}^F)_p C_{P_i}}{4\pi r_{P_i}^2 h_{H_i}}} - 1} \right\}$$

49

Correlations exist for h_{H_i} for evaporating droplets. Ref. 10 gives:

$$(Nu)_H = \frac{2 h_{H_i} r_{p_i}}{k_i} = 2 + 0.6 (P_r)^{1/3} (R_e)^{1/2}$$

50

Equation 50 can be considered the best available correlation under a specified range of conditions. For example, Eq. 50 correlates the Nusselt No. with the Prandtl and Reynolds No's. for the following range of conditions:

$$0 < R_e < 200$$

$$80°F < T_g < 400°F,$$ for droplets of water, and various

hydrocarbons evaporating into air. Therefore, the application of Eq. 50 to the severe conditions which may exist in the present problem must be performed with reservation. It will be assumed that in any case, the basic features of the flow field are retained when correlations of this kind are applied.

Mass Transfer: The analogy between the transfer of heat and mass permits us to express the evaporation rate in manner which parallels the development for the heat transfer. Thus, we define a film coefficient for mass transfer, h_{D_i}, such that:

$$\frac{\dot{W}_{v_i}^F}{N_{i}} = h_{D_i} A_i \left(\rho_{v_{i_{T_p}}} - \rho_{v_i} \right)$$

51

In virtue of the similarity between heat and mass transfer when they occur in separate flow fields, we may expect a correlation for h_{D_i} similar to that for h_{H_i} . Ref. 10 gives:

$$(Nu)_M \;=\; \frac{2\,h_{D_i}\,r_{p_i}}{D_i} \;=\; 2 + 0.6\,(Sc_i)^{1/3}\,(Re_i)^{1/2} \qquad\qquad 52$$

where the Schmidt No. replaces the Prandtl No. in **Eq.** 50 for the heat transfer coefficient.

It should be noted that **Eq.** 51 cannot predict the onset of condensation. The onset of condensation, or nucleation depends on the presence of (1) foreigh impurities which may be in the form of previously condensed substances and (2) clusters of molecules formed of the species under consideration. When only nuclei of the second kind are present the situation is refered to as self-nucleation. In either case, there is a critical nucleus size required above which the droplet continues to grow. Approximate microscropic analysis for critical droplet size and for subsequent droplet growth are given in Ref. 5 and 12. These relations depend on knowledge of surface tension(or surface free energy in the case of solids) for which little is known particularly at the low temperatures of present interest. We will purposely delay specific analysis relating to nucleation and non-equilibrium condensation on the grounds that the mixing process of present interest will probably tend to be in thermodynamic equilibrium. The basis for this assumption rests on the fact the mixing region is boundary layer like and therefore is not subjected to strong streamwise temperature gradients.

The departure from phase equilibrium in supersonic and hypersonic wind
tunnels depends on the existence of severe streamwise temperature gradients
(Ref. 8). A discussion of multicomponent phase equilibrium is given in
section IV.

Viscous Stress: In virtue of assumption (4) the transport of mass, momentum
and energy due to random motion is limited to the gas phase. The pressure
tensor is given by:

$$\underline{\underline{\pi}} = -P_g \underline{\underline{\delta}} + \underline{\underline{\tau}}_g \qquad 53$$

where, $\underline{\underline{\tau}}_g \equiv$ viscous stress tensor

we take the usual Newtonian description for $\underline{\underline{\tau}}_g$ given by:

$$\underline{\underline{\tau}}_g = 2\mu_g \left[\frac{1}{2}\left(\nabla^* \underline{V}_g + \nabla \underline{V}_g \right) \right] - \frac{2}{3}\mu_g \nabla \cdot \underline{V}_g \underline{\underline{\delta}} \qquad 54$$

where μ_g is the absolute viscosity of the gas phase mixture and can be represent-
ed in terms of the gas concentrations of each of the species by (Ref. 13)

$$\mu_g = \sum_i \frac{\mu_i}{1 + \frac{W_i}{W_g Y_{v_i}} \sum_{\substack{j \\ j \neq i}} \frac{W_g}{W_j} Y_j \phi_{ij}} \qquad 55$$

where,

$$\Phi_{ij} = \frac{\left[1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2} \left(\frac{W_j}{W_i}\right)^{1/4}\right]^2}{\frac{4}{\sqrt{2}}\left[1 + \frac{W_i}{W_j}\right]^{1/2}}$$

56

and

$$\mu_i = A_i'\left(T_g\right)^{\omega_i}$$

57

Heat Conduction: Thermal conductivity, as in the case of viscosity, derives from the random motion of the gas phase. Assuming Fourier's Law, we have:

$$\underline{q}_g = -k_g \nabla T_g$$

58

where k_g is the thermal conductivity of the gas phase mixture.

Diffusion: Here, as in the description of viscosity and thermal conductivity, diffusion occurs only in the gas-phase. We assume Fick's Law for the diffusion of the gaseous species which is given by:

$$\underline{j}_{vi} = -\rho_g D_{ij} \nabla Y_{vi}$$

59

where D_{ij} is the binary diffusion coefficient. In general, calculations will be made for specified Prandtl and Lewis No.'s so that there is no present need for

explicit relations for K_g and D_{ij}.

Relations 37c, 48, 51, 54, 58 and 59 complete the description of the rate processes. We have, for the moment, omitted a specific discussion of finite rate chemistry in order to focus our attention on the two-phase problem. The inclusion of chemical reactions requires statements for the $\dot{W}_{vi}^{c}$'s (Ref. 14).

We have mentioned under our discussion of evaporation rates that phase equilibrium may play an important role in the mixing process. It is, therefore, instructive to consider the relations which are applicable in the limiting case of multicomponent phase equilibrium.

IV. MULTICOMPONENT PHASE EQUILIBRIUM:

Classical developments on multicomponent phase equilibrium may be found in Ref's. 15, 16 and 17. We shall limit the present discussion to ideal mixtures for which the activity coefficients are identically equal to unity. Further, we shall assume the fugacites are equal to the pressures. The non-ideality of mixtures as expressed thru the activity coefficients and fugacities must be determined by means external to classical thermodynamics. These quantities are determined, in general, by experimental means. There appear to be no available results for the conditions of present interest. It should be noted, however, that the approximation regarding the fugacities is quite reasonable by virtue of the low pressures under consideration.

Thus, for the ideal mixture composed of perfect gases and condensed phases we define a vaporization equilibrium constant given by:

$$K_{fi} = \frac{\overline{Y_i}}{\overline{X_i}} \qquad\qquad 60$$

where the bar indicates <u>mole</u> fraction. The vaporization equilibrium constant, K_{fi}, is a function of the mixture temperature for given total pressure, i.e.

$$K_{fi} = \frac{P_{si}}{P} \qquad\qquad 61$$

where,

$$\log P_{si} = a_i + \frac{b_i}{T}$$

$$\sum_i \overline{Y_i} = 1$$
$$\sum_i \overline{X_i} = 1 \qquad\qquad 62$$

The total molar concentration of a given species is defined by:

$$\bar{\beta}_i = \frac{\overline{Y_i}\,\bar{\rho}_g + \overline{X_i}\,\bar{\rho}_p}{\bar{\rho}_m} \qquad 63$$

where $\bar{\rho}_m = \bar{\rho}_g + \bar{\rho}_p$ and the bar indicates a molar density, where,

$$\bar{\rho}_g = \sum_i \bar{\rho}_{vi} \qquad 64$$

and

$$\bar{\rho}_p = \sum_i \bar{\rho}_{pi}$$

The degree of vaporization for the mixture is given by:

$$3 = \frac{\bar{\rho}_g}{\bar{\rho}_m} \qquad 65$$

so that Eq. 63 may be written:

$$\bar{\beta}_i = \overline{Y_i}\,3 + \overline{X_i}\,(1-3) \qquad 66$$

or with the aid of Eq. 60;

$$\bar{\beta}_i = \overline{Y_i}\,3 + \frac{\overline{Y_i}}{K_{fi}}\,(1-3) \qquad 67a$$

$$= \overline{X_i}\,K_{fi}\,3 + \overline{X_i}\,(1-3) \qquad 67b$$

Thus, Eq. 67a gives:

$$\overline{Y_i} = \frac{\overline{\beta_i} \, K_{f_i}}{1 + \zeta (K_{f_i} - 1)} \qquad \text{68a}$$

and Eq. 67b gives:

$$\overline{X_i} = \frac{\overline{\beta_i}}{1 + \zeta (K_{f_i} - 1)} \qquad \text{68b}$$

with the aid of Eq's. 62, Eq. 68a and b may be combined to give:

$$\sum_i \frac{\overline{\beta_i}}{\frac{1}{K_{f_i} - 1} + \zeta} \qquad \text{69}$$

Thus, if the total concentration ($\bar{B}_i$) of each species and the mixture temperature are known the concentration distribution of each species is determined. The degree of vaporization is obtained thru Eq. 69 and the gas-phase and condensed-phase concentrations are obtained thru Eq. 68a and b, respectively. For purposes of reference we have the additional relations for the total molar concentrations:

$$\overline{\beta_i} = \overline{\beta_{i_p}} + \overline{\beta_{i_g}} \qquad \text{70}$$

where

$$\overline{\beta_{ip}} = (1-\zeta) \overline{X_i} \qquad\qquad 71a$$

and

$$\overline{\beta_{ig}} = \zeta \overline{Y_i} \qquad\qquad 71b$$

In terms of total mass fractions, we have:

$$W_m = \frac{1}{\sum_i \frac{\beta_i}{W_i}} \qquad\qquad 72$$

where,

$$\overline{\beta_i} = \beta_i \frac{W_m}{W_i} \qquad\qquad 73$$

This analysis implies that each droplet in the condensed phase is a mixture of all condensing species. This would also be true in the case of non-equilibrium condensation or evaporation. Thus, as previously mentioned in the development of the conservation equations for the individual condensed species, the interpretation of these equations must be consistent with the manner in which condensation and evaporation is considered to take place. If each species i is considered to condense into droplets of species i is then the representation of the conservation equations for the individual species requires no interpretation. If, on the other hand, condensation and evaporation occur in accordance with the above equilibrium case, then there will exist only one kind of droplet composed

of all i condensing or evaporation species. In this case, the 3i condensed phase conservations are replaced by 3 condensed phase equations for mass, momentum and energy. There will be a single droplet velocity and temperature. The properties of the condensed phase will be given by:

$$\rho_P = \sum_i \rho_{Pi} \qquad 74$$

$$(C_P)_P = \frac{1}{\rho_P} \sum_i (C_P)_i \rho_{Pi} \qquad 75$$

The evaporation rate for the condensed phase will be given by:

$$\dot{W}_V = \sum_i \dot{W}_{Vi} \qquad 76$$

where

$$\dot{W}_{Vi} = X_i \dot{W}_V \qquad 77$$

Eq. 77 is required for the gas-phase species conservation equations. The droplet drag force and heat convection are also represented by single relations. Specific details of this discussion depend on the particular assumptions made with each case under consideration. This point is discussed in the following application.

V. APPLICATION TO CHEMICALLY FROZEN AXISYMMETRIC JET IN PHASE EQUILIBRIUM

In order to establish limits regarding the presence of a condensed phase we consider the flow to be in equilibrium. The existence of temperature and velocity equilibrium is an assumption based on the condition that the condensed phase is in the form of a cloud of small droplets. If the droplets are small then the heat convection and drag force are large and the resulting temperature and velocity lags will be small. Thus, the presence of small particles is an inherent condition in the equilibrium assumption. Surface tension effects are also neglected. The surface tension plays the governing role in determining the degree of supersaturation which occurs prior to condensation. This effect is primarily limited to the nucleation process where the nucleus size is of molecular dimensions (ref. 12). This effect on the non-equilibrium condensation decreases exponentially with the inverse of the droplet radius. In the adsence of severe streamwise velocity and temperature gradients which is characteristic of the present mixing process, the assumption regarding equilibrium condensation of air appears to be a reasonable first approximation for the major portion of the flow field.

The phase equilibrium of hydrogen requires that the condensed fraction flash to vapor on entering the atmosphere. This equilibrium require-ment is perhaps the limiting assumption in the present example particularly at the higher condensed phase concentrations (up to .45 in present calculations).

In any case, effects of the above assumptions on the flow field decrease as the mass fraction of condensed phase decreases. Thus, we consider the present calculation as a guide to the more complex physical phenomena actually

occuring and interpret the results as quantatively accurate for small mass fraction of condensed phase, and qualitatively descriptive for other configurations.

Governing Equations :

In accordance with the above discussion, the governing equations 27 thru 33 reduce to the following system for the axisymmetric jet Fig. 1 with gas phase Prandtl and Lewis No.'s all equal to unity. These equations are taken to be identical in form for both laminar and turbulent flow with mean turbulent quantities replacing their laminar counterparts .

Continuity:

Global:

$$\frac{\partial \rho_m u r}{\partial x} + \frac{\partial \rho_m v r}{\partial r} = 0 \tag{78}$$

Species:

$$\rho_m u \frac{\partial \beta_i}{\partial x} + \rho_m v \frac{\partial \beta_i}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} r K \frac{\partial \beta_i}{\partial r} \tag{79}$$

Momentum:

$$\rho_m u \frac{\partial u}{\partial x} + \rho_m v \frac{\partial u}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} r K \frac{\partial u}{\partial r} \tag{80}$$

Energy:

$$\rho_m u \frac{\partial H_m}{\partial x} + \rho_m v \frac{\partial H_m}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} r K \frac{\partial H_m}{\partial r} \tag{81}$$

The appropriate boundary and initial conditions for a jet of radius a are:

for $x = 0$, $\quad 0 \leq r < a$

$$u = u_j \quad , \; v = 0 \quad , \; H_m = H_j \quad , \; \beta_{O_2} = \beta_{N_2} = 0$$

$$\beta_{H_2} = 1$$

for

$$x = 0 \quad , \; r > 0$$

$$u = u_e \quad , \; v = 0 \quad , \; H_m = H_e \quad , \; \beta_{O_2} = \beta_{O_2 e} , \; \beta_{N_2} = \beta_{N_2 e} , \; \beta_{H_2} = 0$$

$$x \geq 0$$

$$\lim_{r \to \infty} H = H_e \; , \; u = u_e \; , \; v = 0 \; , \; \beta_{O_2} = \beta_{O_2 e} \; , \; \beta_{N_2} = \beta_{N_2 e} \; , \; \beta_{H_2} = 0$$

with the regularity condition applied along the jet centerline.

for laminar flow we have:

$$k = \mu_g$$

and for turbulent flow we have:

$$k = (\epsilon \rho)_m$$

where ϵ is the eddy viscosity coefficient.

In virtue of the unity Prandtl and Lewis No.'s , similarity in the equations for β_i , u and H_m exists. Further, since the boundary conditions are similar the system admits Crocco relations for H_m and the β_i 's, i.e. H_m and β_i are linearly dependent on the velocity, u. Thus, the problem reduces to that of determining the solution for the velocity distribution. This together with equations of state and appropriate phase equilibrium relations fully determine

the problem.

The solution for u is more readily handled in a corresponding incompressible plane. Following Ref. 18 we introduce the following stream function:

$$\rho_m u r = \rho_e u_e \psi \psi_r$$

$$-\rho_m v r = \rho_e u_e \psi \psi_x \qquad\qquad 82$$

Introducing Von Mises tranformation, i.e. x, r → x, Ψ where,

$$r^2 = \int_0^\psi \frac{2\rho_e u_e}{\rho_m u} \psi' d\psi' \qquad\qquad 83$$

and applying a modified Oseen approximation in form,

$$\frac{\mu_g \rho_m r^2 u}{\rho_e^2 u_e^2 \psi^2} \cong f(x) \qquad\qquad 84$$

where the additional transformation

$$\xi = \int_0^x \frac{f(x')}{\psi_j} dx' \qquad\qquad 85$$

is introduced, the momentum equation becomes:

$$\frac{\partial v}{\partial \xi} = \frac{\psi_j}{\psi} \frac{\partial}{\partial \psi} \left[\psi \frac{\partial v}{\partial \psi} \right] \qquad\qquad 86$$

where,

$$\psi_j = a \left(\frac{\rho_j u_j}{\rho_e u_e} \right)^{1/2} \quad ; \quad \upsilon = \frac{u}{u_e}$$

87

Following Libby (Ref. 14), for laminar flow the approximation function $f(x)$ is evaluated along the jet centerline yielding the inverse transformation:

$$\frac{x}{\psi_j} = \int_0^{\xi} \frac{\rho_e u_e}{(\mu_9)_t} d\xi'$$

88

For turbulent flow a model suitable under present conditions is:*

$$f(x)_t = \frac{n \, r_{1/2}}{u_e} (u_e - u_{\xi})$$

89

where $r_{1/2}$ is the "half radius" defined by:

$$(u)_{r_{1/2}} = \frac{1}{2} \left(u_e + u_{\xi} \right)$$

90

and n is the Prandtl mixing length constant.

The inverse transformation then becomes:

$$\frac{x_t}{\psi_j} = \int_0^{\xi} \frac{1}{f(x)_t} d\xi'$$

91

---

* Note: This model does not predict reasonable results under other conditions: For example, cases where $U_j = 1$. However, the modified eddy viscosity model applied in Ref. 4 is not suitable under present conditions.

The initial and boundary conditions on the momentum equation become:

$$U(0, \psi) = U_j \qquad ; \qquad 0 < \psi < \psi_j$$

$$= 1 \qquad ; \qquad \psi > \psi_j$$

and

$$\lim_{\psi \to \infty} U(\xi, \psi) \to 1$$

With the regularity condition applied along the jet centerline, $\psi = 0$.

The solution of the momentum equation is given by the offset circular probability function P;

$$P = \frac{1-U}{1-U_j} = \frac{\psi_j}{2\xi} e^{-\frac{(\psi/\psi_j)^2}{4\xi/\psi_j}} \int_0^1 e^{-\frac{\psi'^2}{4\xi/\psi_j}} I_0\left[\psi'\left(\frac{\psi}{\psi_j}\right)\left(\frac{2\xi}{\psi_j}\right)^{-1}\right] \psi' d\psi' \qquad 92$$

which has been tabulated in Ref. 19.

In order to perform the inverse transformations to the physical plane (Eq. 83 and 88 of 91), the thermodynamic properties must be determined. The stagnation enthalpy is given by:

$$H_m = \frac{H_e(U-U_j) + H_j(1-U)}{1-U_j} = \frac{u^2}{2} + h_m \qquad 93$$

and the total species concentrations are given by:

$$\beta_{O_2} = \beta_{O_2 e} \frac{\upsilon - \upsilon_j'}{1 - \upsilon_j'}$$

$$\beta_{N_2} = \beta_{N_2 e} \frac{\upsilon - \upsilon_j'}{1 - \upsilon_j'}$$

$$\beta_{H_2} = \frac{1 - \upsilon}{1 - \upsilon_j'}$$

94

The Equation of State is given by:

$$P = P_e = \rho_m \left\{ \frac{\beta_{O_2 g}}{W_{O_2}} + \frac{\beta_{N_2 g}}{W_{N_2}} + \frac{\beta_{H_2 g}}{W_{H_2}} \right\} RT$$

95

where,

$$P_{O_2 g} = \rho_m \frac{\beta_{O_2 g}}{W_{O_2}} RT$$

$$P_{N_2 g} = \rho_m \frac{\beta_{N_2 g}}{W_{N_2}} RT$$

$$P_{H_2 g} = \rho_m \frac{\beta_{H_2}}{W_{H_2}} RT$$

96

The stagnation enthalpy is given by:

$$H_m = \frac{u^2}{2} + \beta_{O_2} \left\{ h_{O_2 g} - \frac{\beta_{O_2} - \beta_{O_2 g}}{\beta_{O_2}} L_{O_2} \right\}$$

$$+ \beta_{N_2} \left\{ h_{N_2 g} - \frac{\beta_{N_2} - \beta_{N_2 g}}{\beta_{N_2}} L_{N_2} \right\}$$

$$+ \beta_{H_2} \left\{ h_{H_2} - \frac{\beta_{H_2} - \beta_{H_2 g}}{\beta_{H_2}} L_{H_2} \right\}$$

97

where,

$$h_{ig} = h_{ig}(T)$$ 98

and

$$L_i = L_i(T)$$ 99

The equilibrium conditions used in the present calculation will be an approxima-
tion to the results presented in section IV. We shall consider the partial
pressure of a species in two phases to be equal to the saturation pressure
corresponding to the existing temperature. This is exact when only one of the
species condensed. However, the error is small in virtue of the steep slope of
the vapor-pressure curves. That is, the range of temperature over which two
phases of each species exist in comparable proportions is extremely narrow.
This, coupled with the close similarity between Oxygen and Nitrogen justifies
the assumption.

Thus we have:

Nitrogen:

$$\log_{10} P_{N_2}(mmHg) \cong 7.6589 - \frac{359.093}{T(°K)}$$ 100

Oxygen:

$$\log_{10} P_{O_2}(mmHg) = 9.131 - \frac{482}{T(°K)}$$ 101

where, Eq. 100 is given in Ref. 20 and Eq. 101 is a curve fit of data given in Ref. 21.

Relations 94 thru 101 fully determine the nature of the flow field in the velocity plane and supply the required thermodynamic variables for the transformation to physical coordinates via Eq.'s 83, 88 or 91 and the viscosity relation, Eq. 55.

Method of Solution in the Velocity Plane

The solution in the velocity plane can be carried out for the following given data:

(a) Altitude

(b) Hydrogen tank conditions with an isentropic expansion to atmospheric conditions

(c) Vehicle trajectory i.e. u_e vs Altitude

Now, for each velocity ratio $U_j < U < 1$ the computations proceed in the following manner:

(1) Assume T

(2) Assume O_2 and N_2 exist in two phases so that $P_{N_2} g$ and $P_{O_2} g$ are determined by Eq.'s 100 and 101 respectively.

(3) P_{H_2} is determined by:

$$P_{H_2} = P_e - P_{N_2 g} - P_{O_2 g}$$

(4) β_{O_2} g and β_{N_2} g are determined by Eq.'s 93, i.e. :

$$\beta_{O_2 g} = \frac{P_{O_2 g}}{P_{H_L}} \frac{\beta_{H_L}}{W_{H_L}} W_{O_L}$$

and

$$\beta_{N_2 g} = \frac{P_{N_2 g}}{P_{H_L}} \frac{\beta_{H_L}}{W_{H_L}} W_{N_L}$$

(5) (a) if β_{O_2} g $< \beta_{O_2}$ then assumption (2) for O_2 is valid. Similarly for N_2 .

(b) if β_{O_2} g $> \beta_{O_2}$ then assumption (2) is incorrect and we take all O_2 in the gas phase. Similarly for N_2 .

(6) With (1) and the results of (4) and (5), the stagnation enthalpy must be checked. In Eq. 97 H_m and u are knwon and the β_i's have just been determined. Thus, with (1) we can determine whether the stagnation enthalpy relation is satisfied. If it is not satisfied, a new temperature is assumed, step (1), and the computations are repeated. This procedure is carried out for each velocity ratio U in the range $U_j < U < 1$ corresponding to each set of given date. Calculations were carried out for the following given data:

Altitude (KM)	P_e ATM	T_e (°K)	u_e F.P.S.	H_e 61/gm	H_j Cal/gm	u_j F.P.S.
60	0.000252	254	7330	65$\therefore$	175	2785
40	0.00298	261	4990	340	175	2460
20	0.0545	216	2420	117	175	1880

Additional quantities which were taken as constants in the calculations are:

$$\beta_{O_2}e = 0.232$$

$$\beta_{N_1}e = 0.768$$

$$L_{O_2} \cong 65 \frac{cal.}{gm}$$

$$L_{N_2} \cong 57 \frac{cal.}{gm}$$

Hydrogen fuel tank:

$$T_t = 20.0 \ ^{\circ}K \ sat.$$

$$a = 1 \ inch$$

Thermodynamic properties used in the calculations are given in Ref.'s 20 and 21.

VI. <u>DISCUSSION</u>

The description of the phenomena resulting from the dumping of cryogenic hydrogen into the atmosphere requires a departure from the usual one-dimensional pipe flow models found in the literature for treating two-phase flows. The class of problems of interest depend on mixing for their description and therefore require a multidimensional analysis. Since the present problem involves the mixing into air of cryogenic hydrogen with a normal boiling point substantially lower than the air we will, in general, encounter small condensed phase mass fractions. Thus, in such a mixing process, the condensed phase will form a dilute suspension in the gas phase. In the present work a model is developed for treating the flow of a dilute suspension of condensing and evaporating components. Velocity and temperature lags between the phases are accounted for in terms of appropriate momentum and energy interaction parameters. Evaporation and condensation is accounted for in terms of appropriate mass transfer and the associated momentum and energy transfer parameters. In addition to these inter-phase transfers we have gas phase viscosity, thermal conductivity, and diffusion of the gas phase components. The description of the inter-phase tranport phenomena poses a substantial problem in itself. There is a general lack of fundamental constitutive relations to account for the simultaneous occurrence of the above discussed inter-phase rate processes. This is particularly true of the nucleation and condensation processes at the low temperatures of current interest. In any case, this area requires much additional work. Thus, it is necessary to adopt a semiempirical approach which in general will be qualitatively valid and in certain limiting cases will

provide quantitatively valid results.

In the present numerical example the boundary conditions are such that the flow will be chemically frozen. This removes the added complication of rate chemistry and permits this preliminary analysis to focus on multi-phase effects. In particular, the analysis and numerical results for a diffusion controlled axisymmetric jet are presented. Fig's. 1 thru 4j show the jet geometry and the distributions of the pertinent variables, respectively. Fig. 1 is a schematic representation of the axisymmetric jet showing the inner cone composed essentially of undisturbed two-phase hydrogen. In crossing the cone boundary, the hydrogen flashes to vapor in accordance with the equilibrium assumption. The remaining figures show the radial and axial distributions of mixture mass fractions of condensed phase and gas phase components. In addition, temperature and velocity distributions are presented. These results are for the altitudes of 20, 40 and 60 KM. There are some general features characteristic of all altitude determinations. We note that the air is completely condensed until certain radial and axial positions are attained. At these points there is a rapid spacewise transition from solid to vapor accompanied by a plateau or an actual decrease in temperature. The rapid phase change is due to the large rate of increase in saturation pressure with temperature. Thus, a point is reached where the local pressure and mixture concentrations cannot support the condensed phase. The energy required for the evaporation is derived from the gas phase and consequently inhibits a temperature increase in this transition zone. A feature of considerable interest is the streamwise extent within which two phases exist. The two limiting cases of laminar and fully

developed turbulent flows have been treated and provided the maximum and

minimum "two-phase lengths", respectively. The long lengths in the laminar

flow are attributed to the low viscosities associated with the low temperatures.

The turbulent model used in the present case provides an eddy viscosity based

strictly on dynamic quantities, i.e. on the velocity difference between the axis

and free stream. This could account for the large $\sim 1000/1$ ratio for the

laminar to turbulent two-phase lengths on the axis. We expect ratios of the

order of $100/1$. In any case, the actual two-phase lengths depend on the degree

to which turbulence has developed. Thus, we can only estimate that for the

present problem two-phase lengths on the order of hundreds of feet can be

expected.

Regarding effects on ignition and combustion of hydrogen we note

that two-phase flow does not exist above $T \cong 50^{\circ}k$. At temperatures of this

magnitude, we cannot expect any chemical activity. This implies that even

for appropriate (high temperature) free stream conditions, the existence of

two-phase flow provides an additional ignition time delay factor. That is, before

ignition occurs re-evaporation must take place where temperature rises are

inhibited. This is characteristic of ignition delay.

It has been pointed out that the equilibrium assumption applied to

the hydrogen is perhaps the limiting assumption in the present jet problem. In

order to asses this assumption a "partial equilibrium" analysis is currently

being programmed for digital computation. In particular, two-phase hydrogen

is injected into an air stream where it assumed that the air condenses in

equilibrium. On the otherhand, the condensed hydrogen particles are allowed to evaporate according to an appropriate rate law. Included in this work will be the effects of small particle evaporation and condensation in rarefied atmospheres pertinent to the high altitude range of present interest. In order to provide an insight into the effect of finite rate evaporation the limiting case of zero interphase mass transfer is shown in Fig. 5 . The details of the partial equilibrium analysis will be available under separate cover at a later date.

REFERENCES

1. Taub, P. A., Slot Injection of Reactive Gases in Laminar Flow With Application to Hydrogen Dumping, GASL Technical Report No. 332, Jan. 1963.

2. Libby, P. A., Schetz, J. A., Approximate Analysis of Slot Injection of a Reactive Gas in Laminar Flow, GASL Technical Report No. 293, Nov. 1962.

3. Libby, P. A., Pergament, H. S., Taub, P., Engineering Estimates of Flow Lengths Associated With the Combustion of Hydrogen-Air Mixtures During a Launch Trajectory, GASL Technical Report No. 330, Dec. 1962.

4. Rosenbaum, H., Axisymmetric Laminar and Turbulent Jets of Hydrogen with Simple Chemistry, GASL Technical Report No. 331, Jan. 1963.

5. Wegener, P. P., and Mack, L. M., Condensation in Supersonic and Hypersonic Wind Tunnels, Advances in Applied Mechanics, Vol. 5, pp. 307-447, 1958.

6. Hirschfelder, Curtiss, and Bird, Molecular Theory of Gases and Liquids, John Wiley and Sons, 1954.

7. Edelman, R. B., The Flow of a Dilute Suspension of Solids in a Laminar Gas Boundary Layer, Doctoral Thesis, Yale University, 1962.

8. Pouring, A. A., An Experimental and Analytical Investigation of Homogeneous Condensation of Water Vapor in Rapid Expansions, Doctoral Thesis, Yale University, 1963 (in preparation)

9. Hermans, J. J., Flow Properties of Disperse Systems, North Holland Publishing Co , pp. 319-322, 1953.

10. Ranz, W. E., and Marshall, W. R. Jr., Evaporation from Drops, Chemical Engineering Progress, Part I, Vol. 48, No. 3, March 1952, pp 141-146 and Part II, Vol. 48, No. 4, April 1952, pp. 173-180.

11. Graves, C.C. and Bahr, D.W., Basic Considerations in the Combustion of Hydrocarbon Fuels in Air, Chapter I, NACA, Report 1300, 1957.

12. Frenkel, J., Kinetic Theory of Liquids, Dover Publishing Co., Chapter 7, 1955.

13. Bromley, L.A. and Wilke, C.R., Viscosity Behavior of Gases, Industrial and Engineering Chemistry, Vol. 43, July 1951.

14. Libby, P.A., Theoretical Analysis of Turbulent Mixing of Reactive Gases with Application to Supersonic Combustion of Hydrogen, A.R.S. Journal, Vol. 32, No. 3, March 1962.

15. Guggenheim, E.A., Thermodynamics, North Holland Publishing Co., Chapter 5 and 7, 1957.

16. Hall, N.A. and Idele, W.E., Engineering Thermodynamics, Prentice-Hall Publishing Co., Chapter 12, 1960.

17. Zemansky, M.W., Heat and Thermodynamics, McGraw-Hill Publishing Co., Chapter 19, 1957.

18. Kleinstein, G., An Approximate Solution for the Axisymmetric Jet of a Laminar Compressible Fluid, Polytechnic Institute of Brooklyn, Sept. 1962.

19. Masters, J.I., Some Applications in Physics of the P. Function, Journal of Chemical Physics, Vol. 23, Oct. 1955.

20. Tables of Thermodynamic Properties of Gases, National Bureau of Standards, Circular 564, Nov. 1955.

21. Mullins, J.C., Ziegler, W.T., and Kirk, B.S., The Thermodynamic Properties of Oxygen From 20° to $100^{\circ}K$, Georgia Institute of Technology, TR-2 (N.B.S. MR-8), March 1, 1962
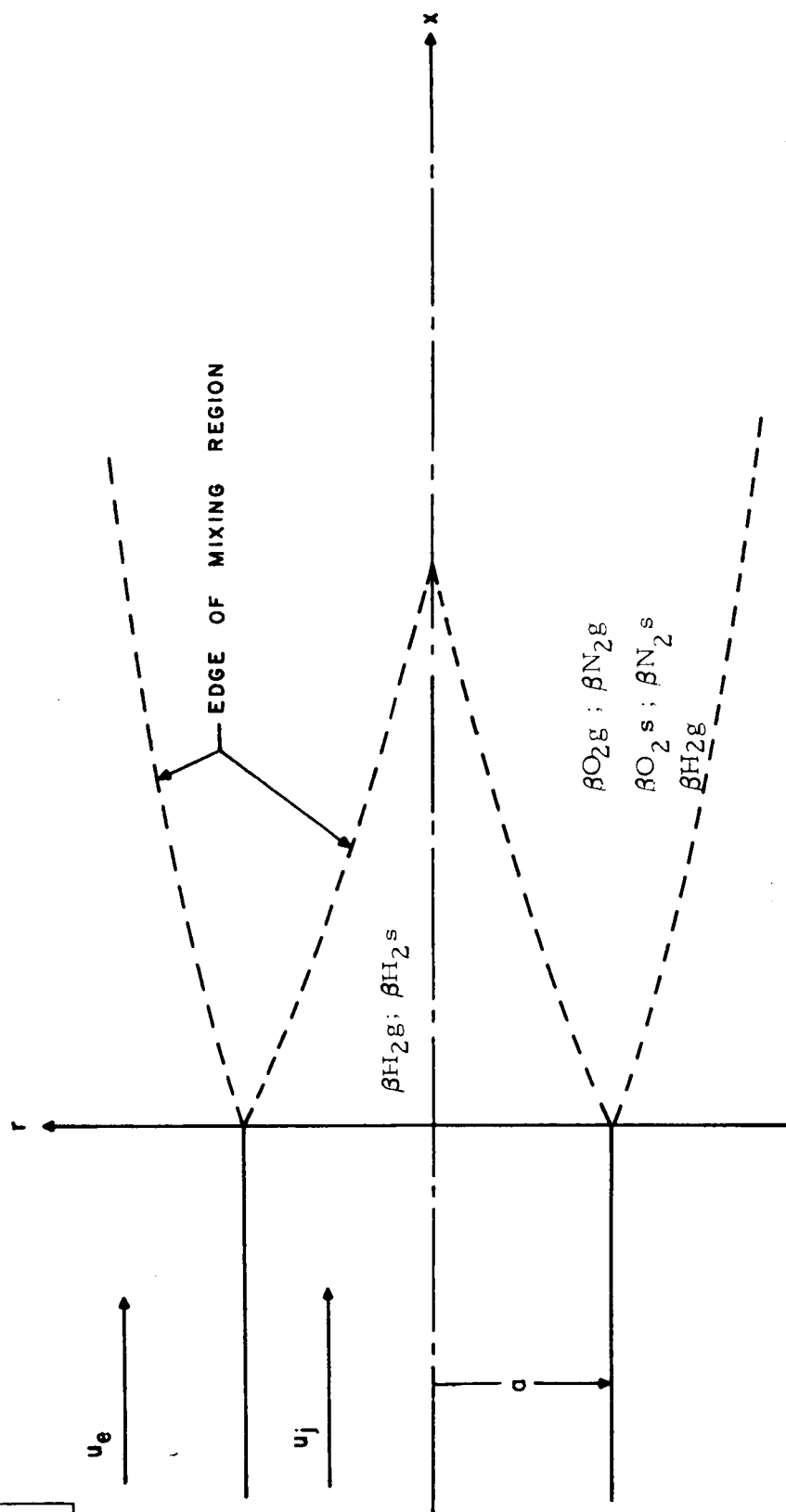
FIG. I SCHEMATIC OF FLOW REGION
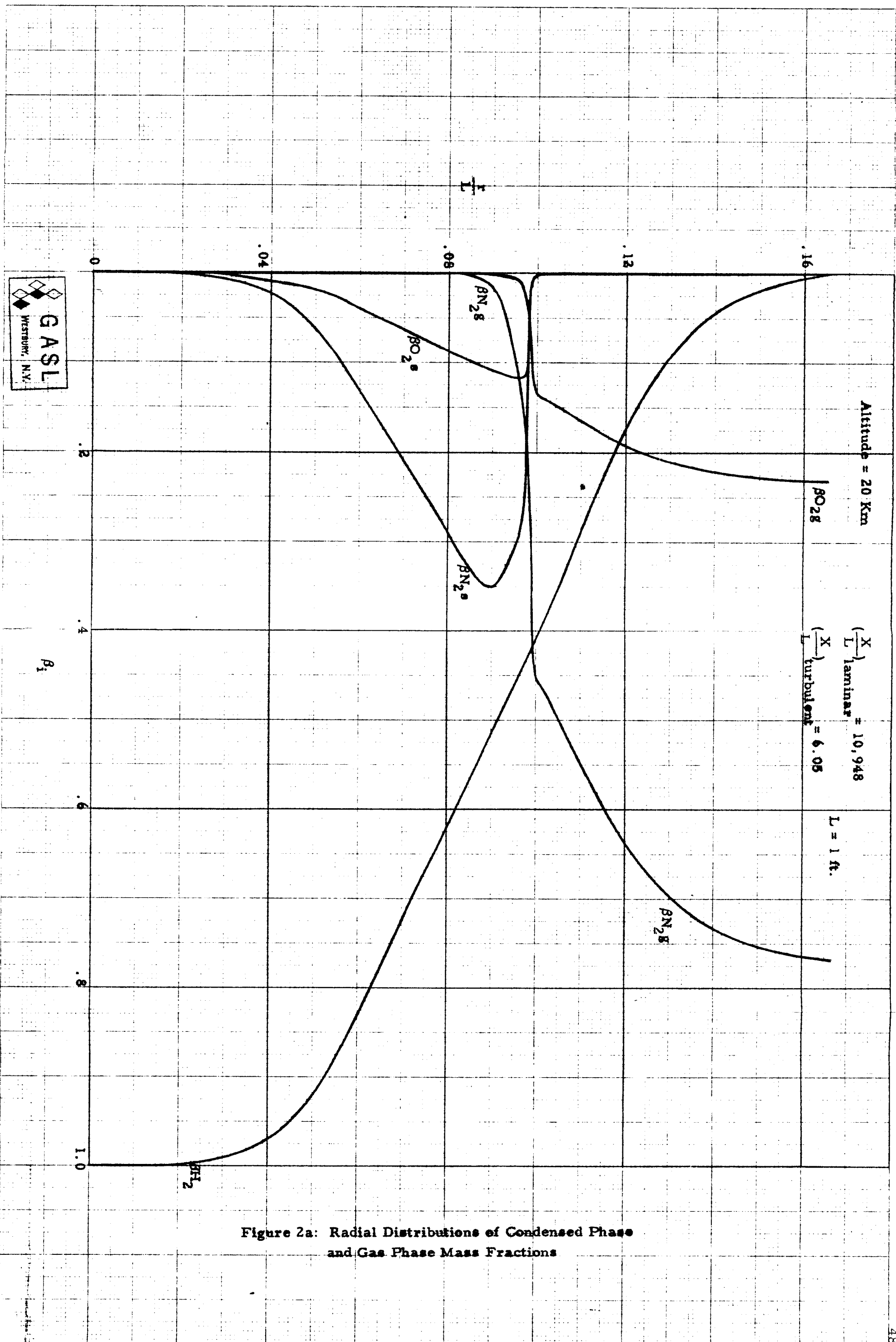
Figure 2a: Radial Distributions of Condensed Phase
and Gas Phase Mass Fractions

Altitude = 20 Km

$\left(\dfrac{X}{L}\right)$ laminar = 10,948

$\left(\dfrac{X}{L}\right)$ turbulent = 6.05

L = 1 ft.
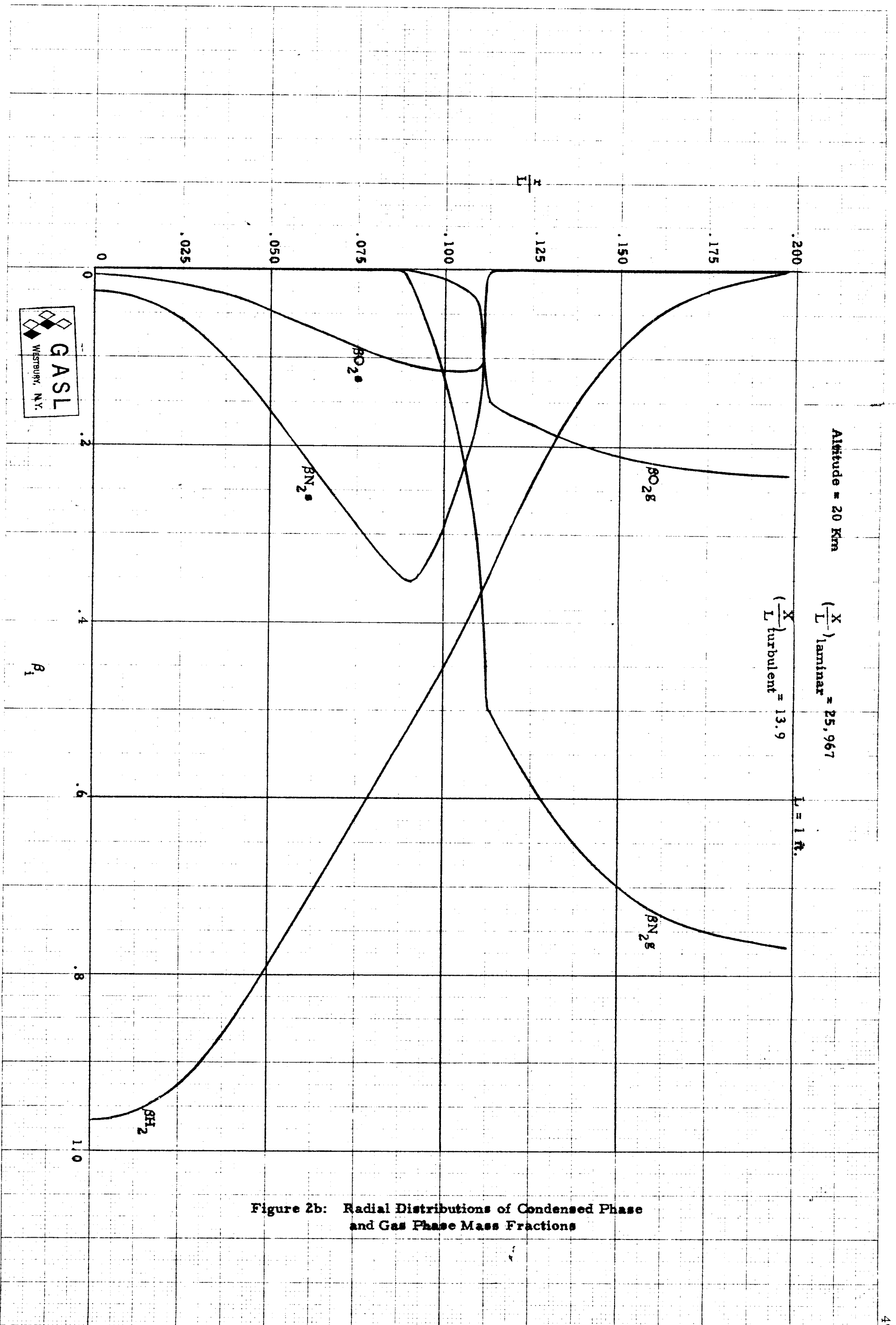
Figure 2b: Radial Distributions of Condensed Phase and Gas Phase Mass Fractions

Altitude = 20 Km

$(\frac{X}{L})_{laminar} = 25,967$

$(\frac{X}{L})_{turbulent} = 13.9$

$L = 1$ ft.
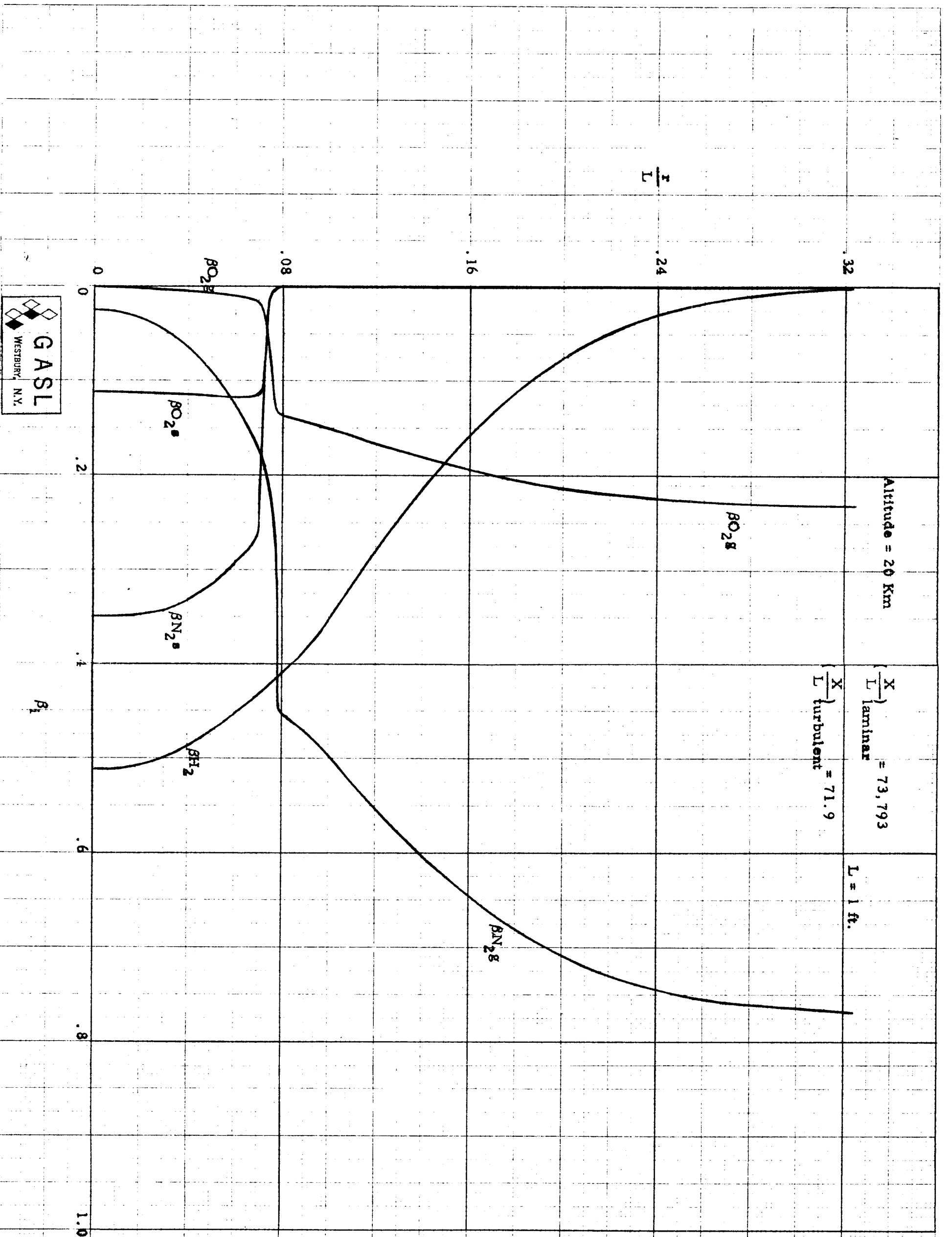
Figure 2c: Radial Distributions of Condensed Phase and Gas Phase Mass Fractions

GASL
WESTBURY, N.Y.

Altitude = 20 Km

$\left(\dfrac{X}{L}\right)_{laminar}$ = 73,793

$\left(\dfrac{X}{L}\right)_{turbulent}$ = 71.9

L = 1 ft.

$\dfrac{r}{L}$

β_i

βO_{2g}

βO_{2s}

βN_{2s}

βH_2

$\beta N_{2}g$

Figure 2d: Radial Distributions of Velocity and Temperature at 20 Km

$$\left(\frac{X}{L}\right)_{laminar} = 10,948$$

$$\left(\frac{X}{L}\right)_{turbulent} = 6.05$$

$\frac{r}{L}$

T/T_e

u/u_e

T/T_e , u/u_e

GASL
WESTBURY, N.Y.
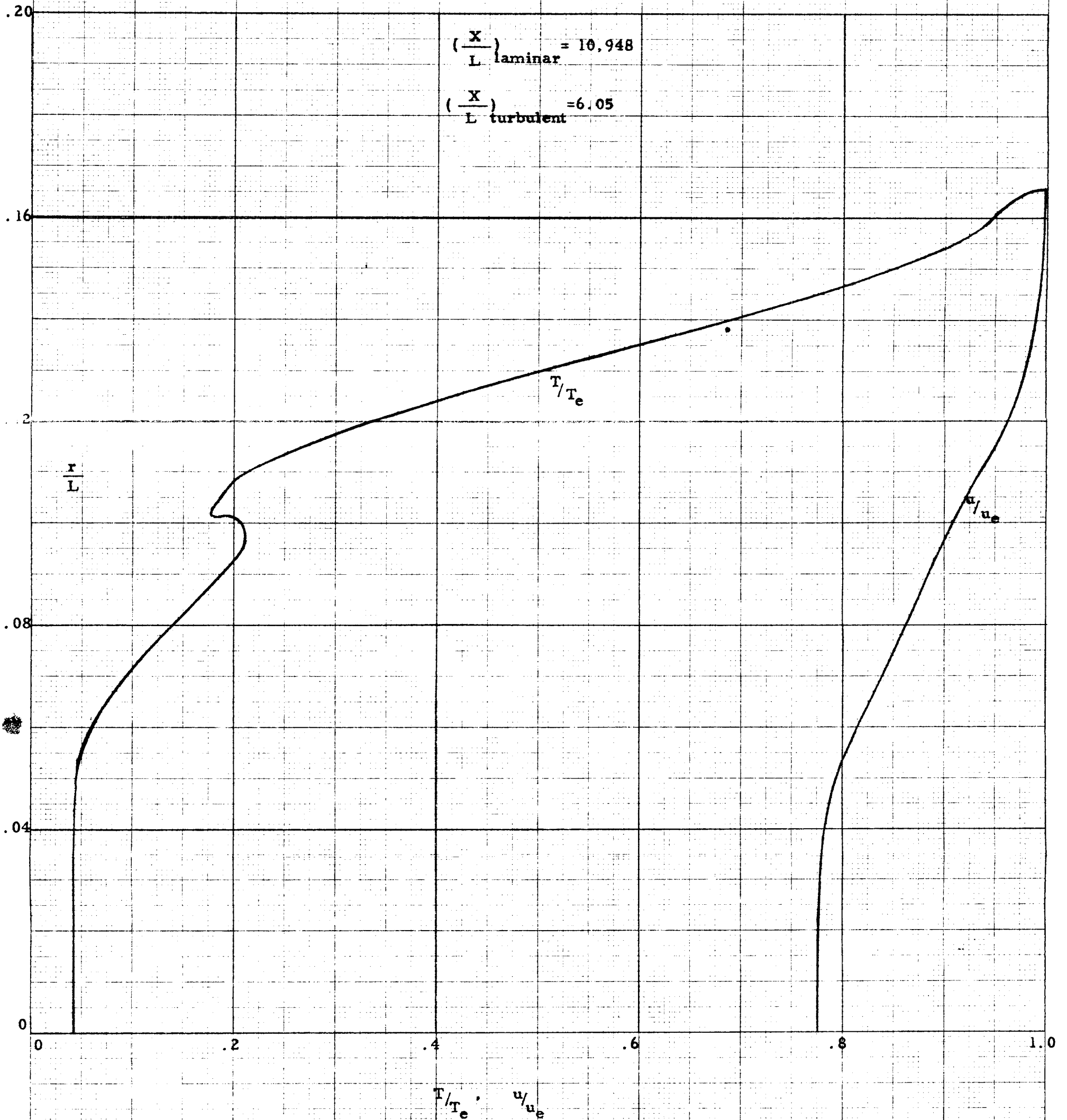
Figure 2e: Radial Distribution of Velocity and Temperature at 20 Km

$$\left(\frac{X}{L}\right)_{laminar} = 25,967$$

$$\left(\frac{X}{L}\right)_{turbulent} = 13.9$$

$$L = 1 \text{ ft.}$$

T/T_e

u/u_e

$\frac{r}{L}$

T/T_e , u/u_e
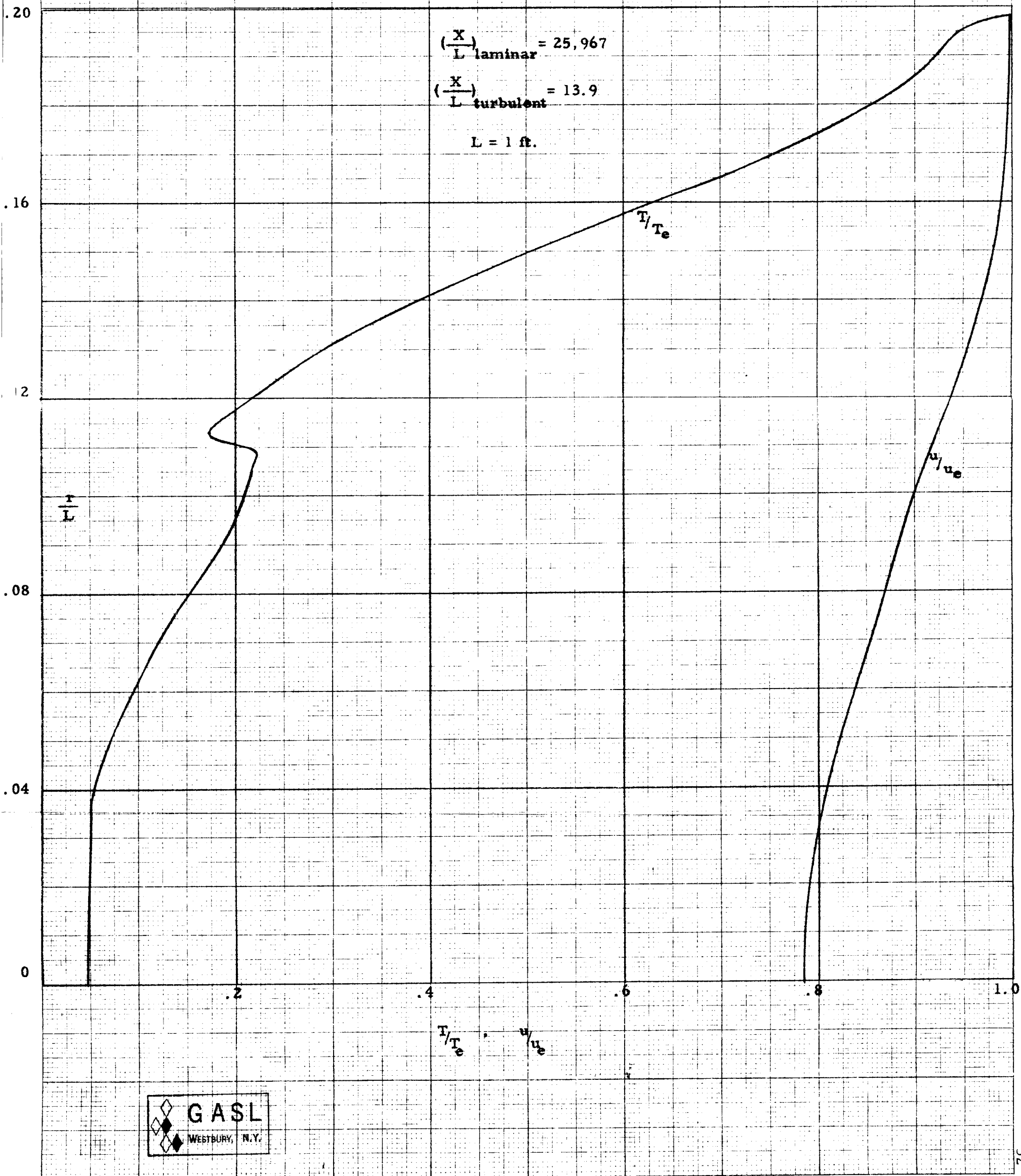
GASL
WESTBURY, N.Y.

Figure 2f: Radial Distribution of Velocity and Temperature at 20 Km
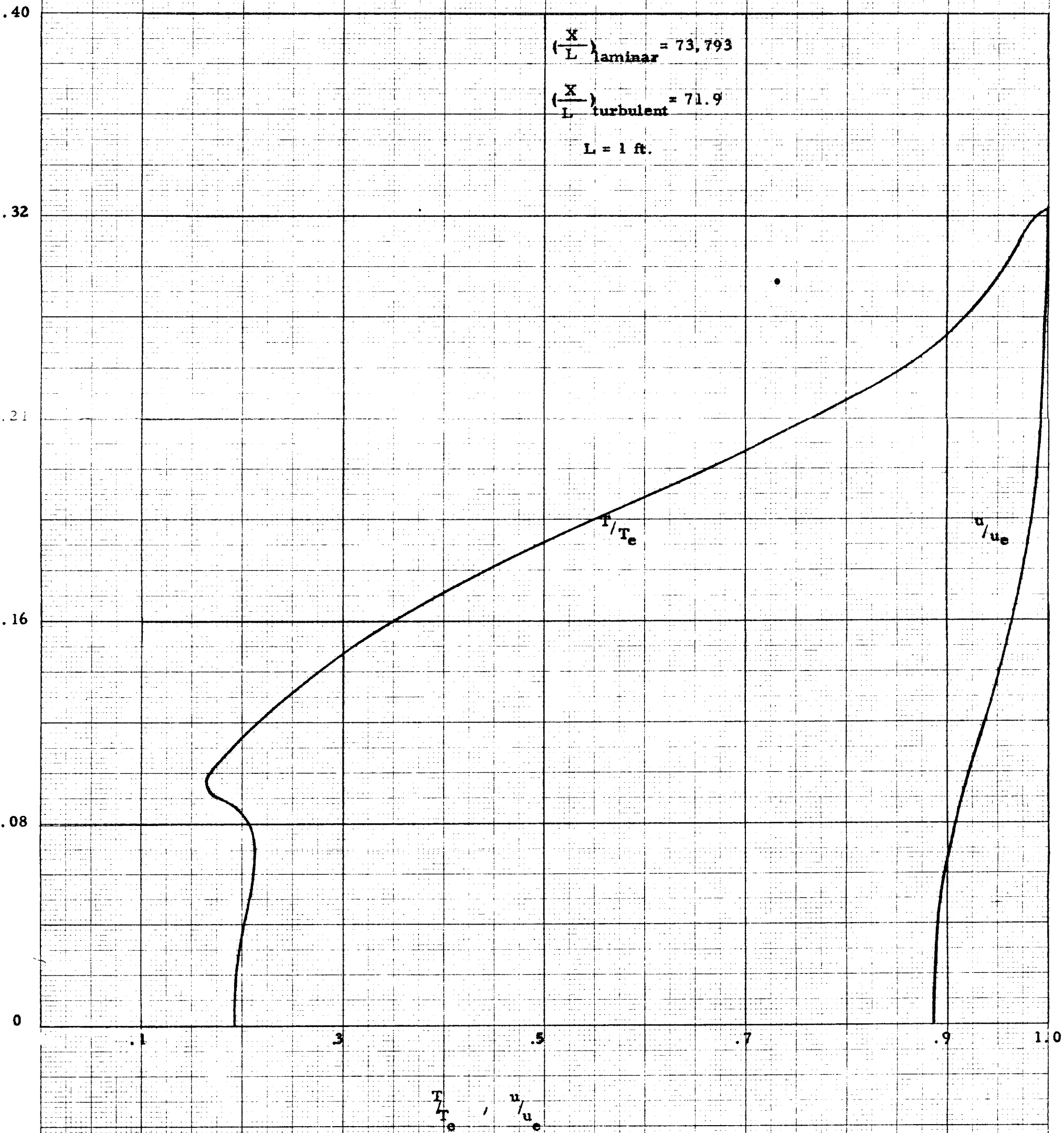
$(\frac{X}{L})_{laminar} = 73,793$

$(\frac{X}{L})_{turbulent} = 71.9$

$L = 1$ ft.

T/T_e

u/u_e

$\frac{T}{T_e}$, $\frac{u}{u_e}$

GASL
WESTBURY, N.Y.

53

Figure 24: Axial Distributions of Condensed Phase and Gas Phase Mass Fraction
Laminar Jet, .20 Km
L = 1 k.
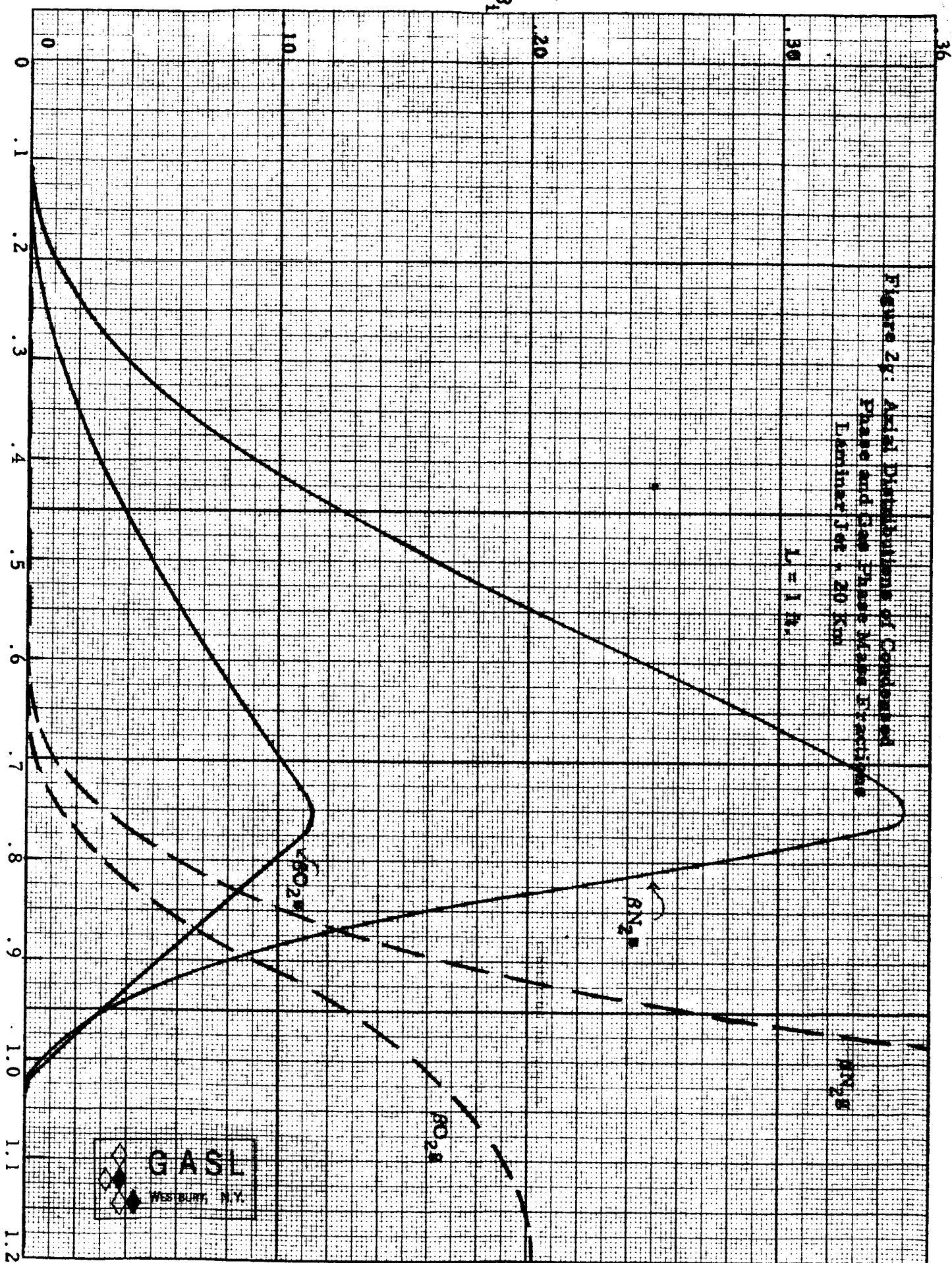
Figure 2b. Axial Distributions of Velocity and Temperature. Laminar Jet. Altitude = 20 Km.
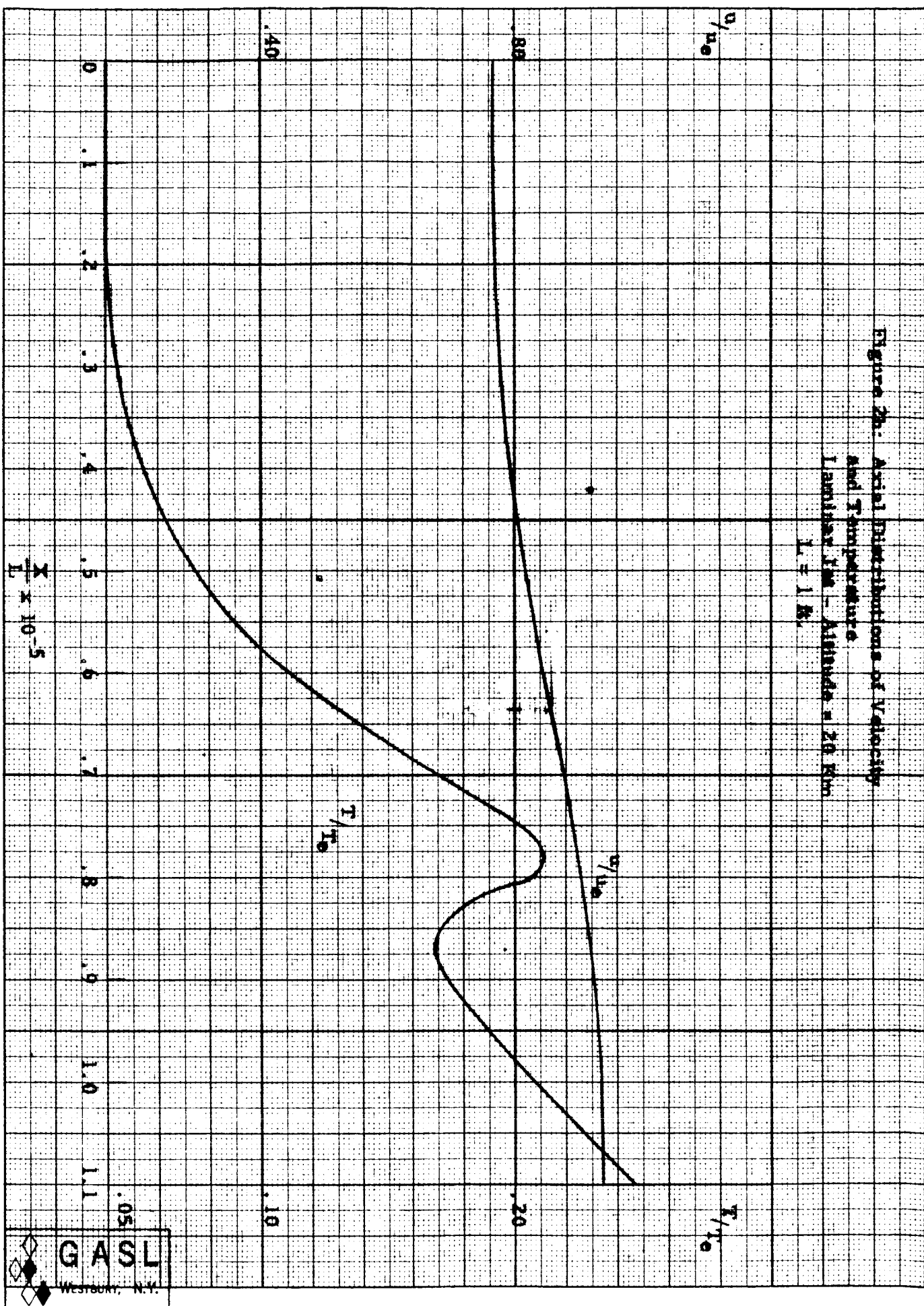
Figure 21: Axial Distributions of Condensed Phase
and Gas Phase Mass Fractions
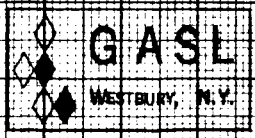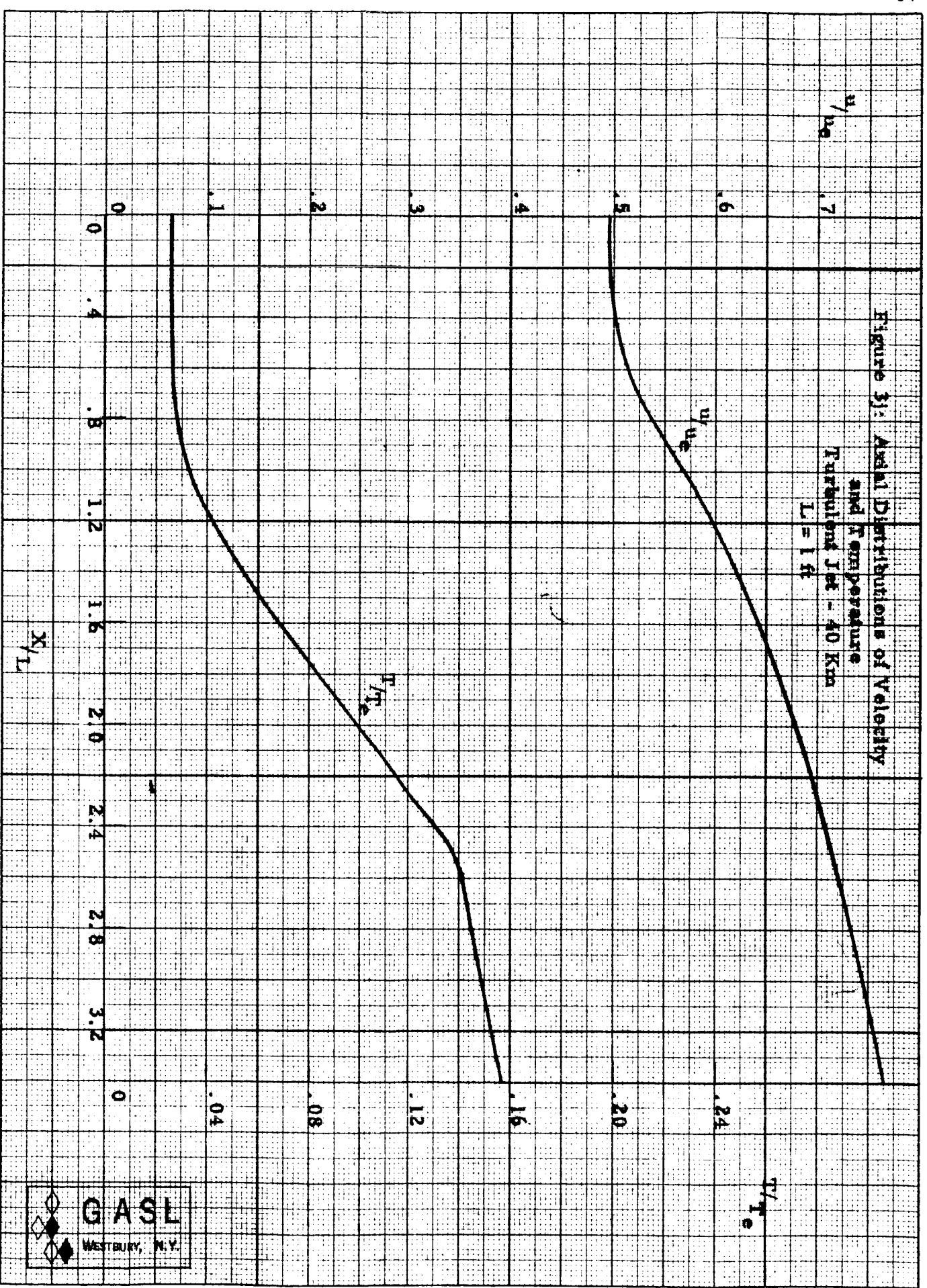Turbulent Jet - 20 Km
L = 1 ft.

Figure 23. Axial Distributions of Velocity and True Temperature
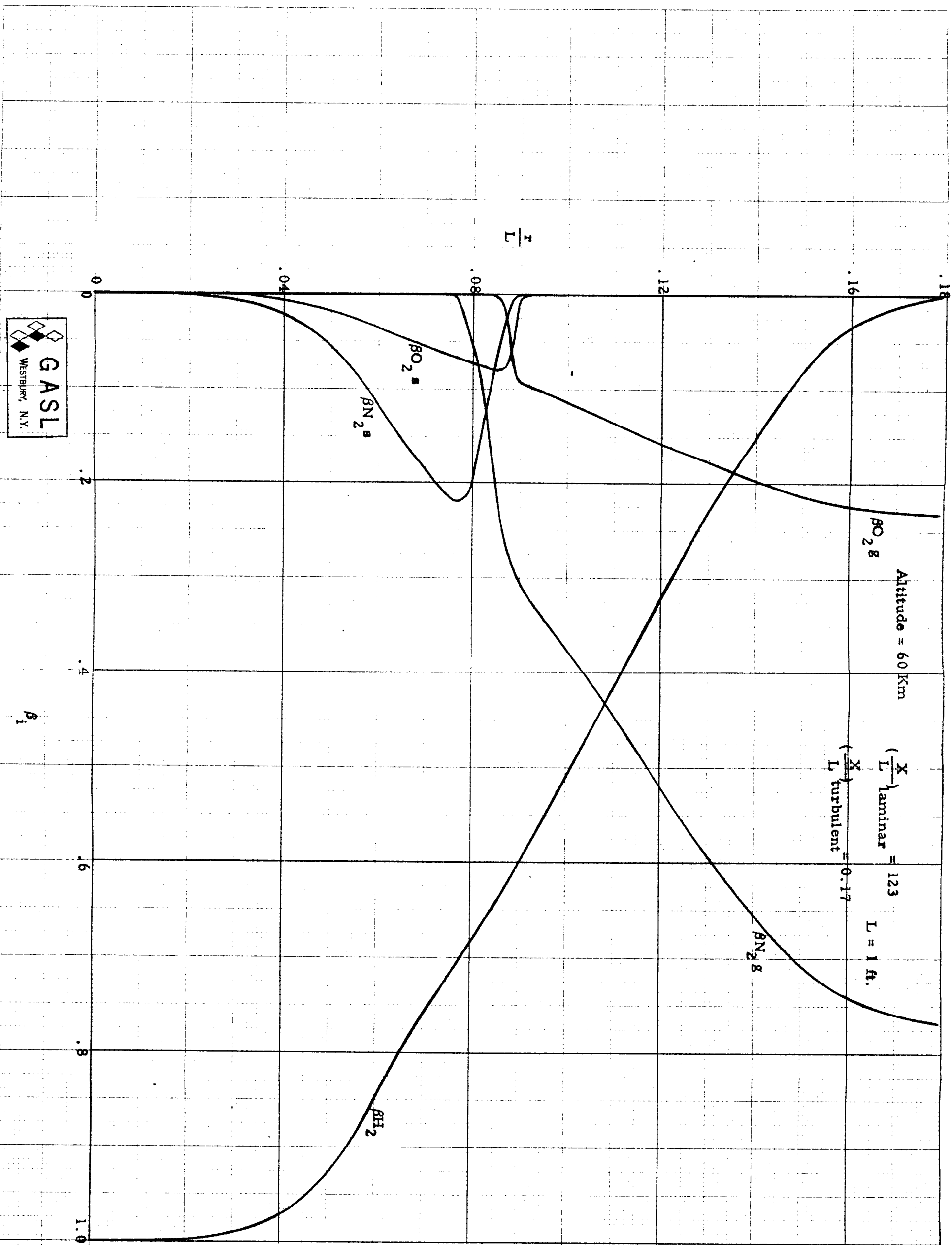
Turbulent Jet-Altitude 20 Km

$L = 1$ ft.
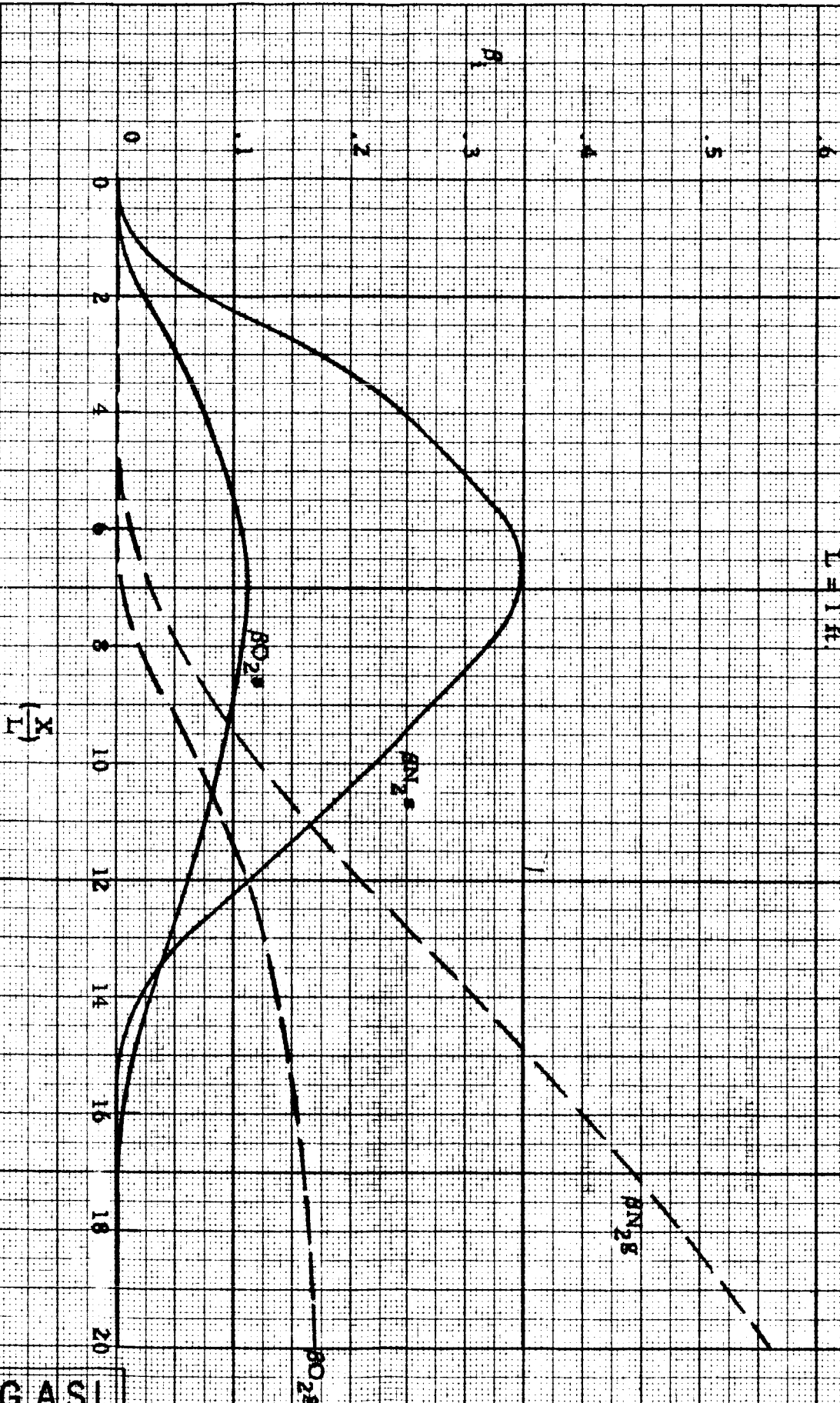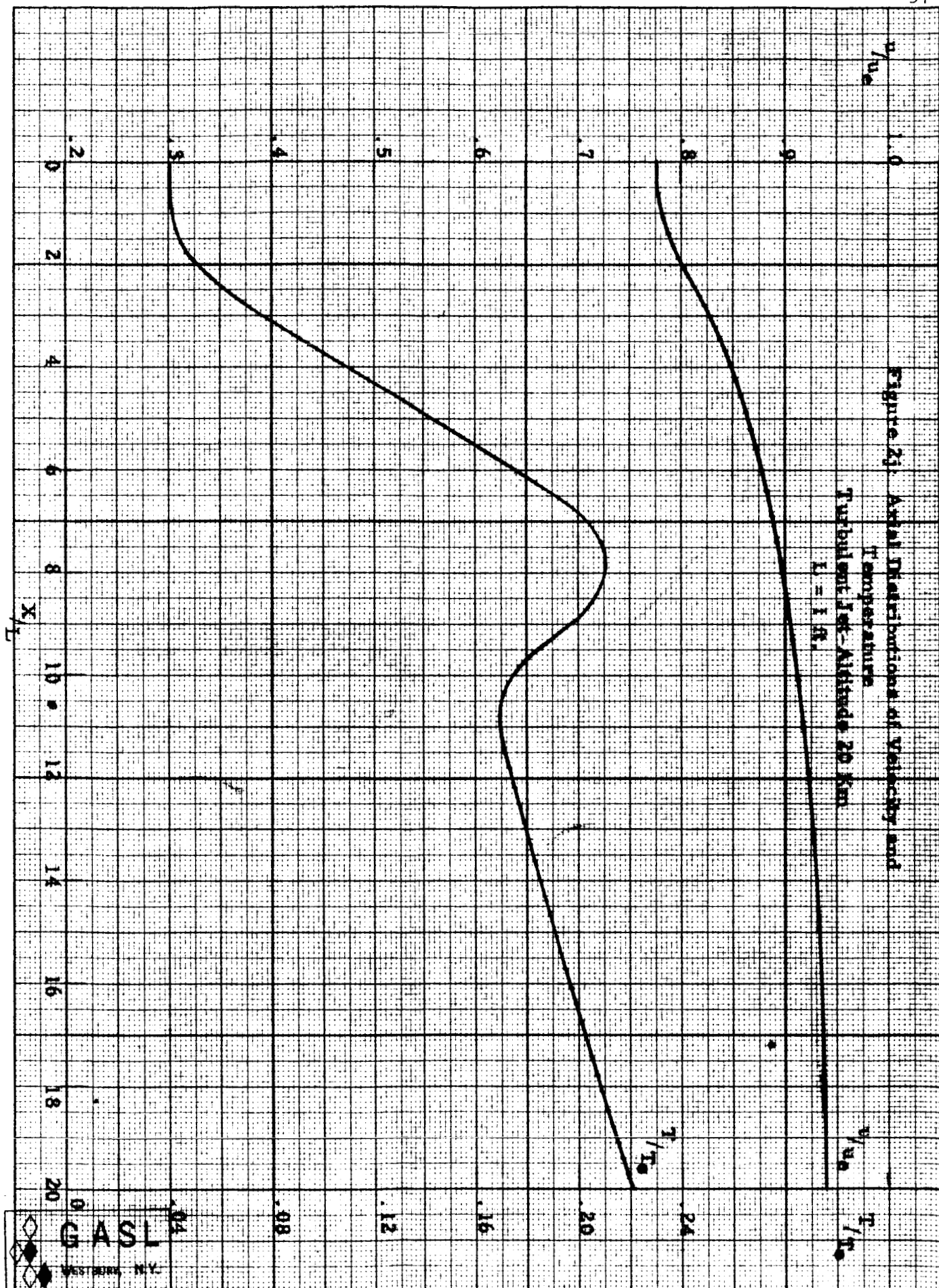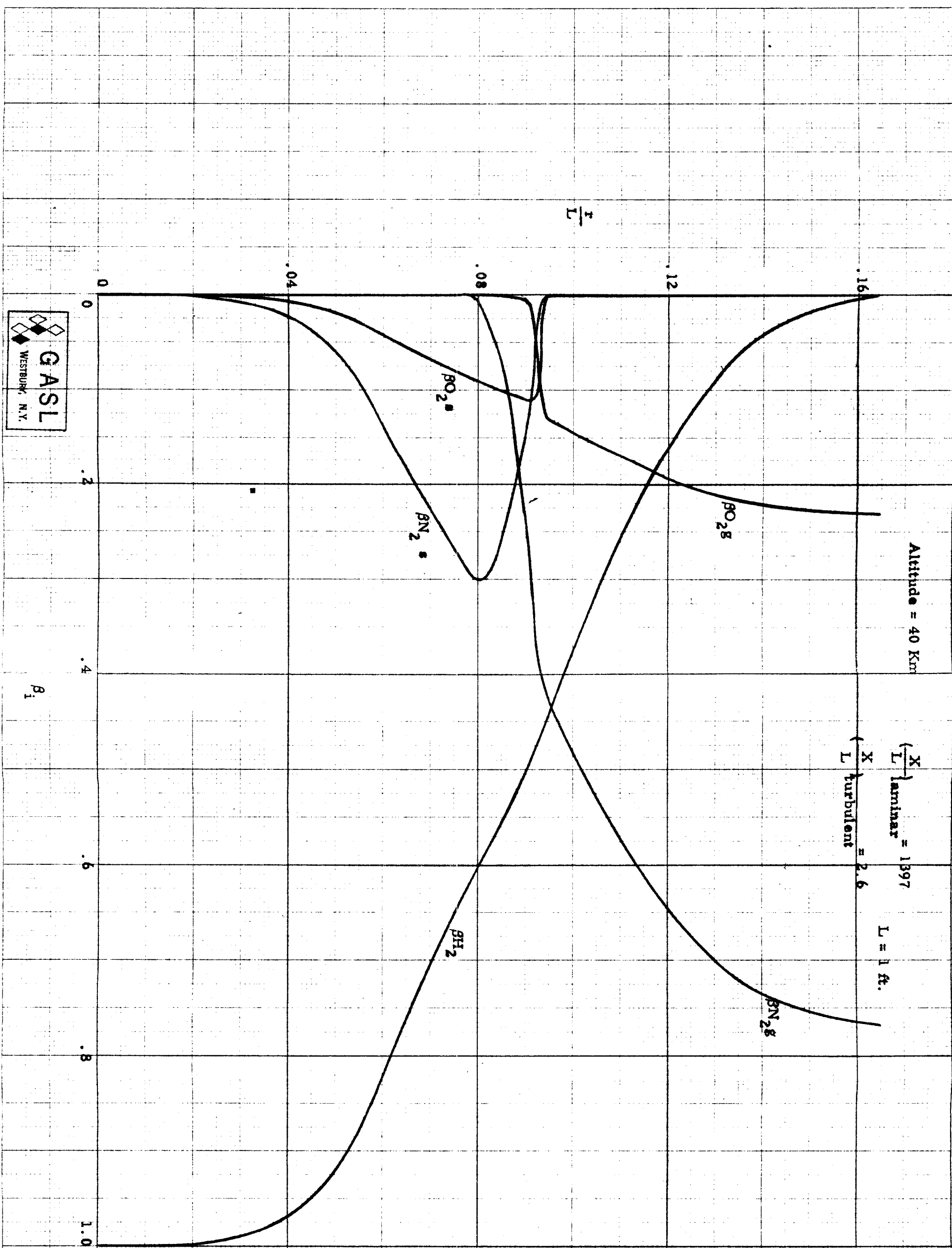
Figure 3a: Radial Distributions of Condensed Phase
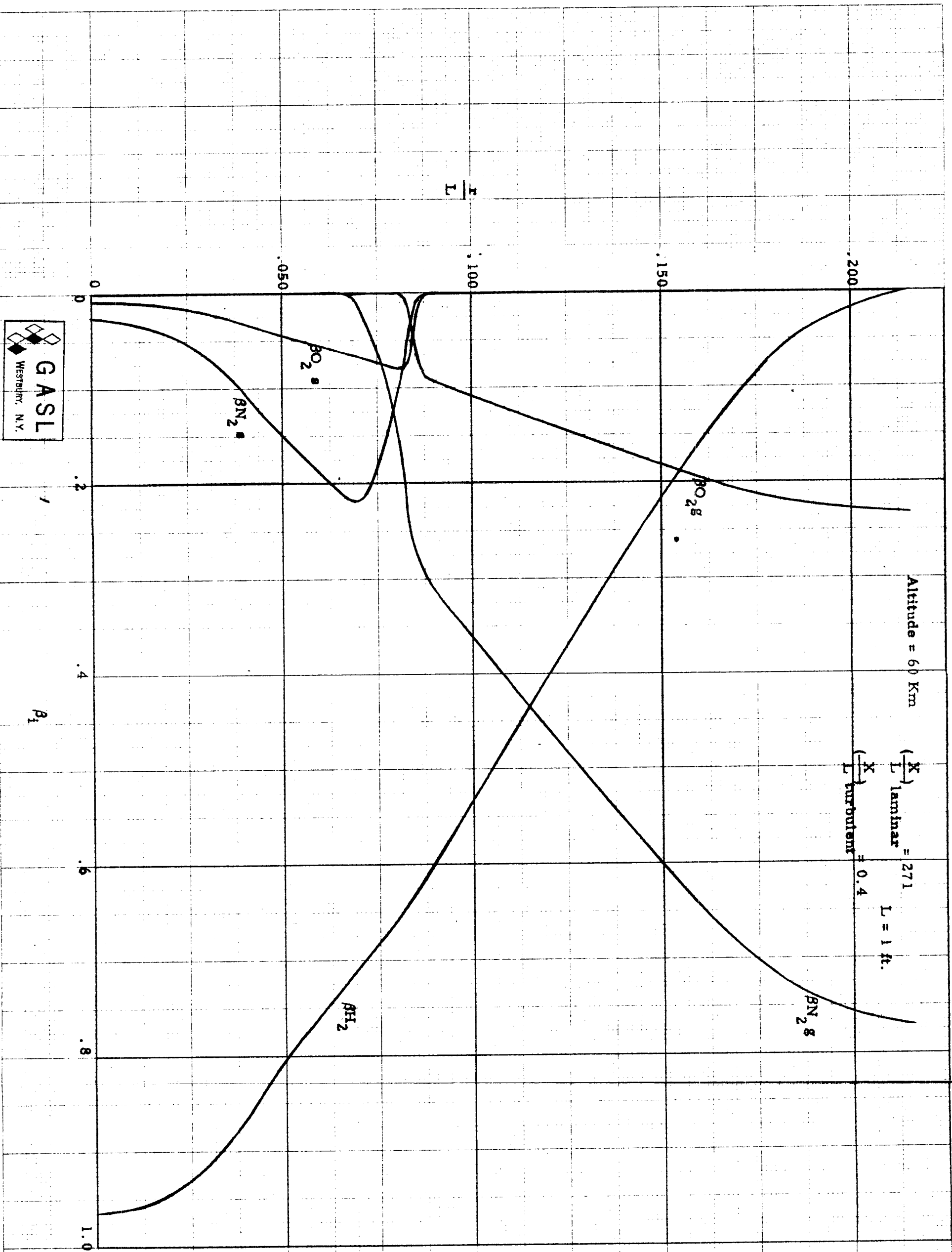and Gas Phase Mass Fractions
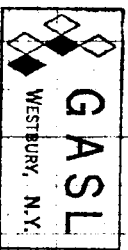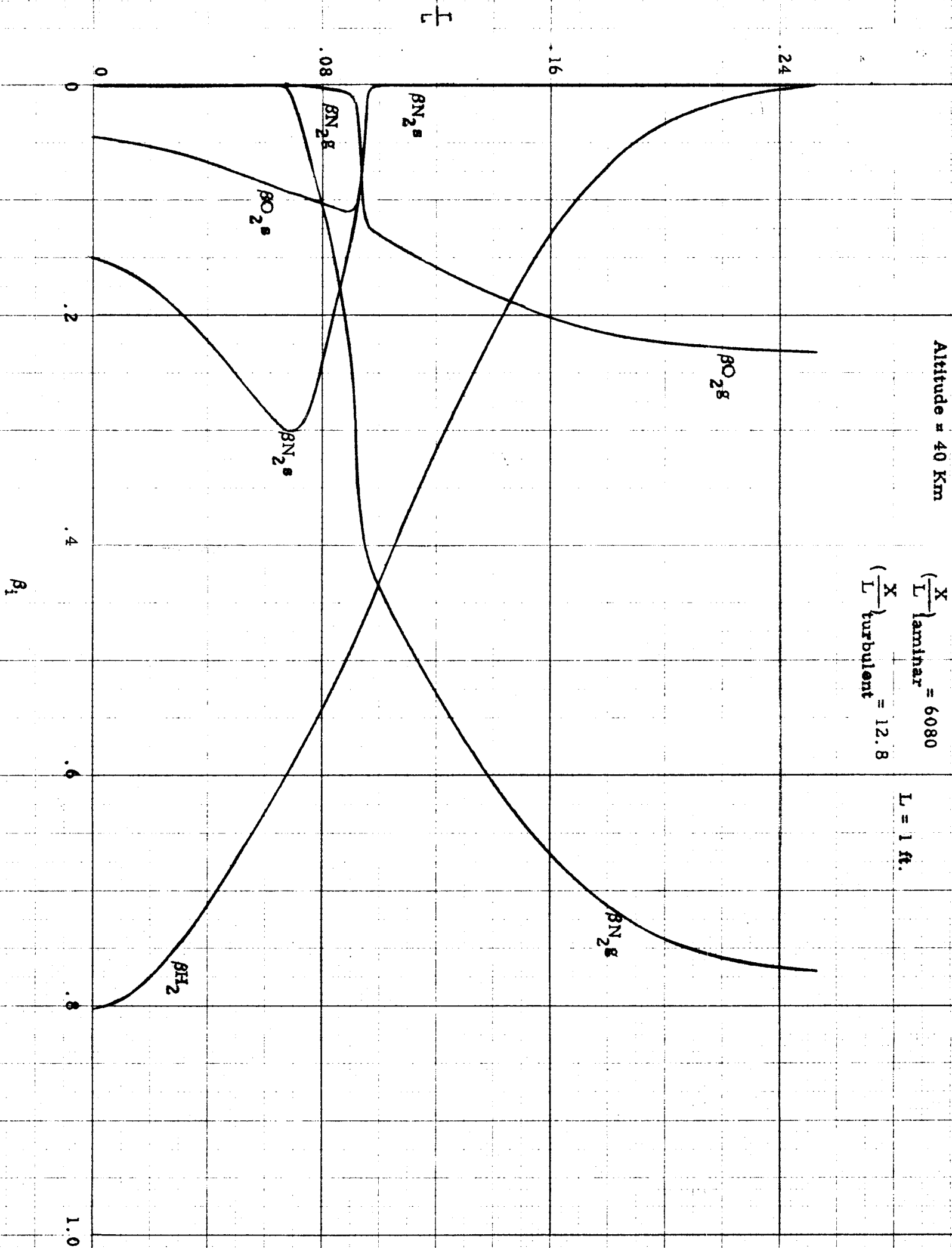
Figure 3b: Radial Distributions of Condensed Phase
and Gas Phase Mass Fractions
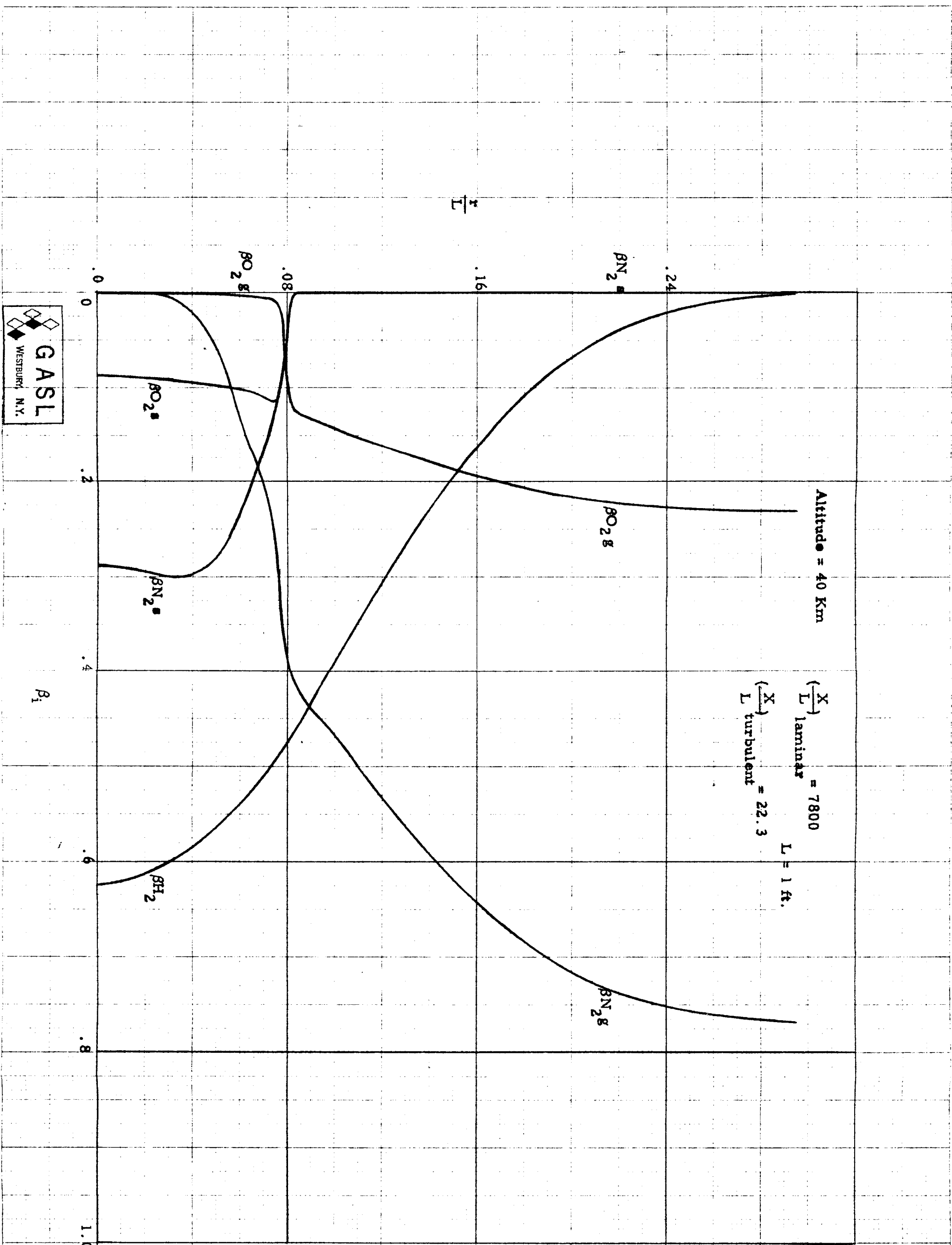
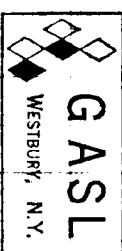Figure 3c: Radial Distributions of Condensed Phase
and Gas Phase Mass Fractions

Altitude = 40 Km

$\left(\dfrac{X}{L}\right)_{laminar} = 7800$ $L = 1$ ft.

$\left(\dfrac{X}{L}\right)_{turbulent} = 22.3$

β_i

$\beta O_2 s$

$\beta N_2 s$

$\beta O_2 g$

$\beta N_2 g$

$\beta N_2 g$

βH_2

$\dfrac{r}{L}$

Figure 3d: Radial Distributions of Velocity and Temperature at 40 Km

$\left(\dfrac{X}{L}\right)_{laminar} = 1397$

$\left(\dfrac{X}{L}\right)_{turbulent} = 2.6$

$L = 1$ ft.

T/T_e

u/u_e

$\dfrac{r}{L}$

$T/T_e \cdot u/u_e$

GASL
WESTBURY, N.Y.
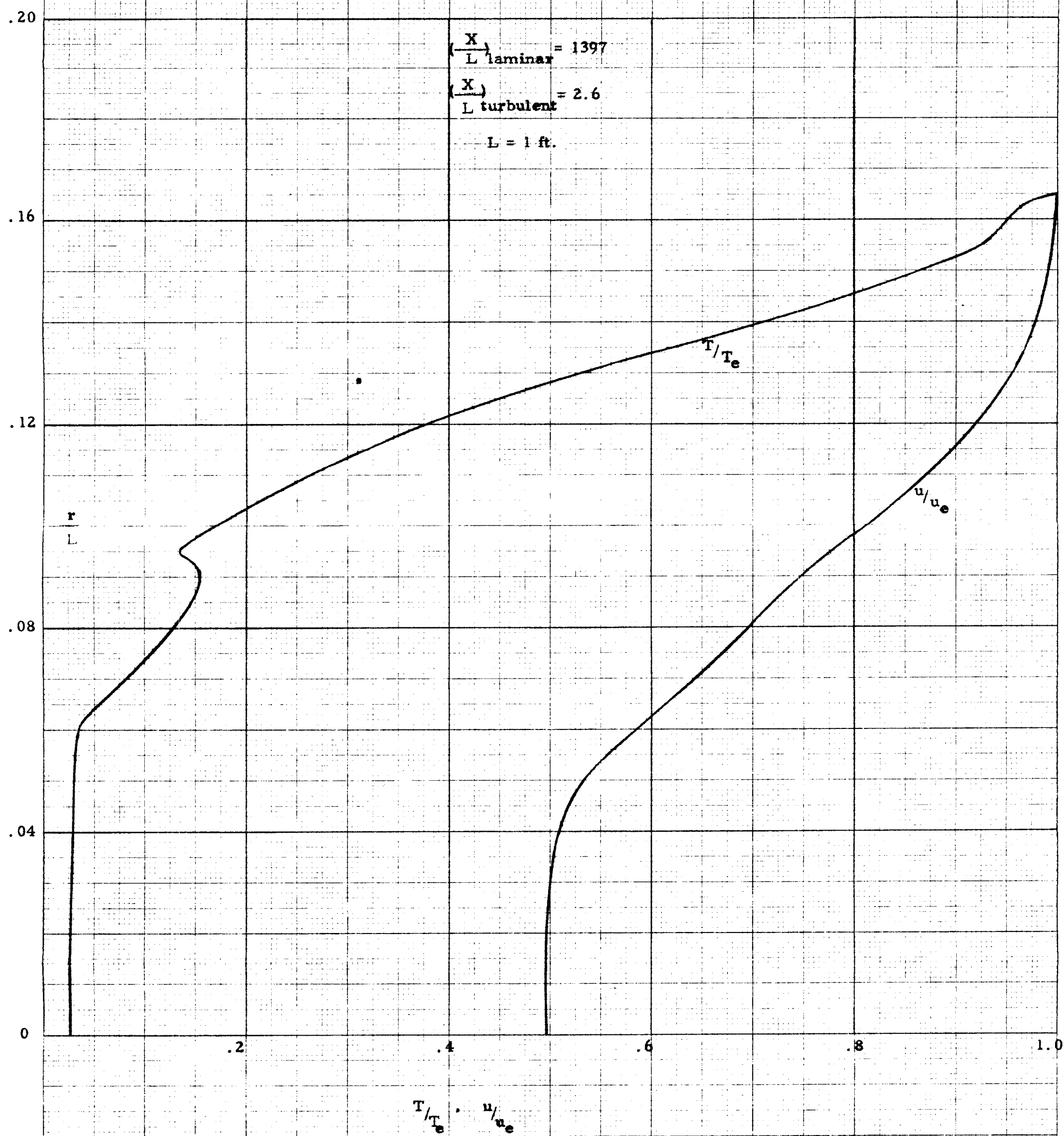
Figure 3e: Radial Distributions of Velocity and Temperature at 40 Km

$\left(\dfrac{X}{L}\right)_{laminar} = 6080$

$\left(\dfrac{X}{L}\right)_{turbulent} = 12.8$

$L = 1$ ft.

$\dfrac{r}{L}$
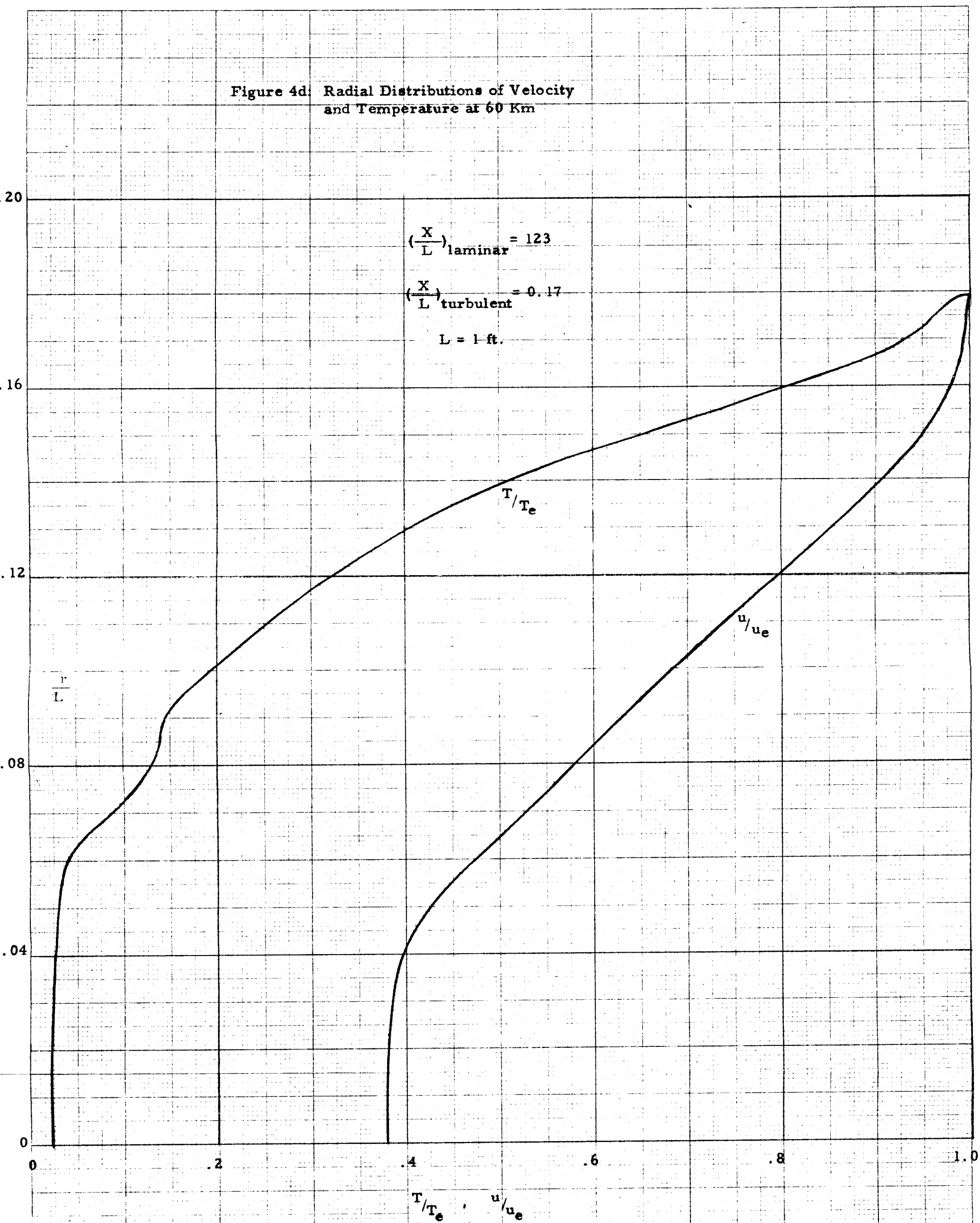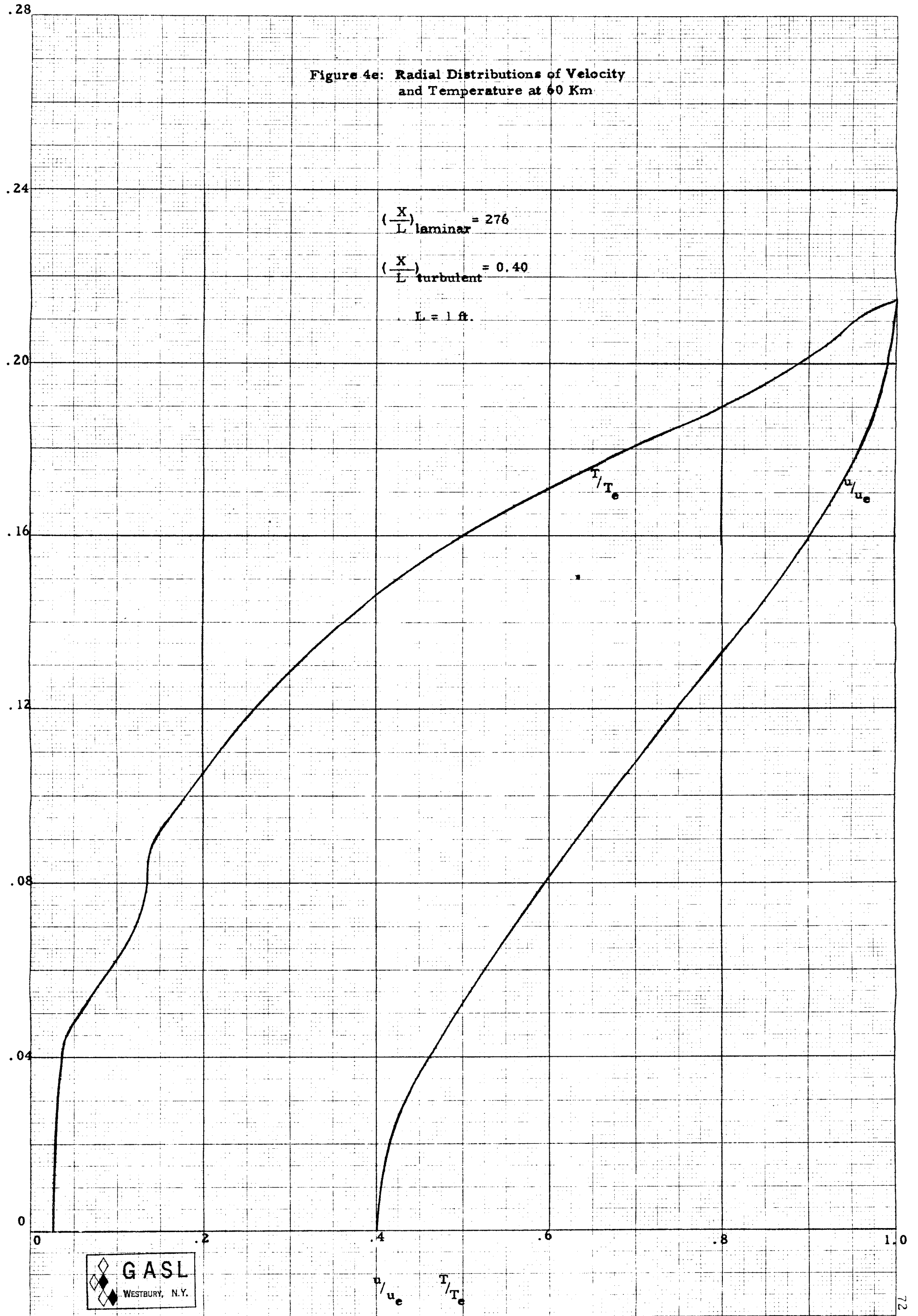
T/T_e

u/u_e

T/T_e , u/u_e

GASL
WESTBURY, N.Y.
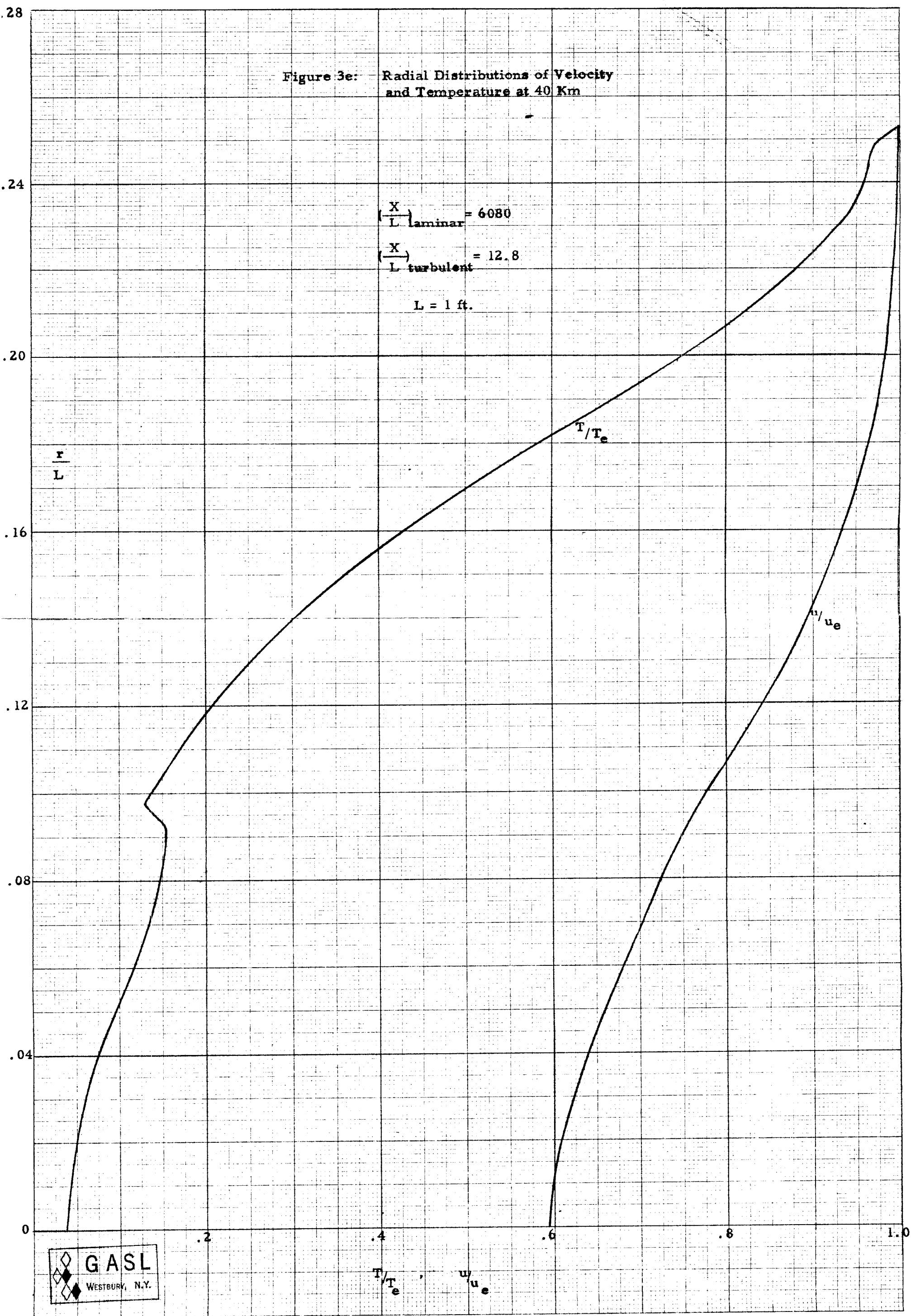
Figure 3f: Radial Distributions of Velocity and Temperature at 40 Km

$$\left(\frac{X}{L}\right)_{laminar} = 7800$$

$$\left(\frac{X}{L}\right)_{turbulent} = 22.3$$

$$L = 1 \text{ ft.}$$

$\frac{r}{L}$

T/T_e

u/u_e

$T/T_e \quad u/u_e$

GASL
WESTBURY, N.Y.

Figure 3: Axial Distribution of Condensed Phase and Gas Phase Mass Fractions
Trailing Jet = 4.0 Km

$L = 1$ ft.

Figure 31: Axial Distribution of Velocity
and Temperature
L = 1 ft.

Figure 3: Axial Distributions of Condensed Phase
And Gas Phase Mass Fractions - Turbulent Jet - 40 Km

L = 1 ft.

Figure 3j: Axial Distributions of Velocity
and Temperature
Turbulent Jet - 40 Km
L = 1 ft

Figure 4a: Radial Distributions of Condensed Phase and Gas Phase Mass Fractions

Altitude = 60 Km

$\left(\frac{X}{L}\right)_{laminar} = 123$ L = 1 ft.

$\left(\frac{X}{L}\right)_{turbulent} = 0.17$

GASL
WESTBURY, N.Y.
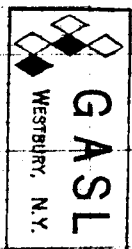
Figure 4b: Radial Distributions of Condensed Phase and Gas Phase Mass Fractions

Figure 4c: Radial Distributions of Condensed Phase
and Gas Phase Mass Fractions

Altitude = 60 Km

$\left(\dfrac{X}{L}\right)_{\text{laminar}} = 443$

$\left(\dfrac{X}{L}\right)_{\text{turbulent}} = 0.8$

$L = 1$ ft.

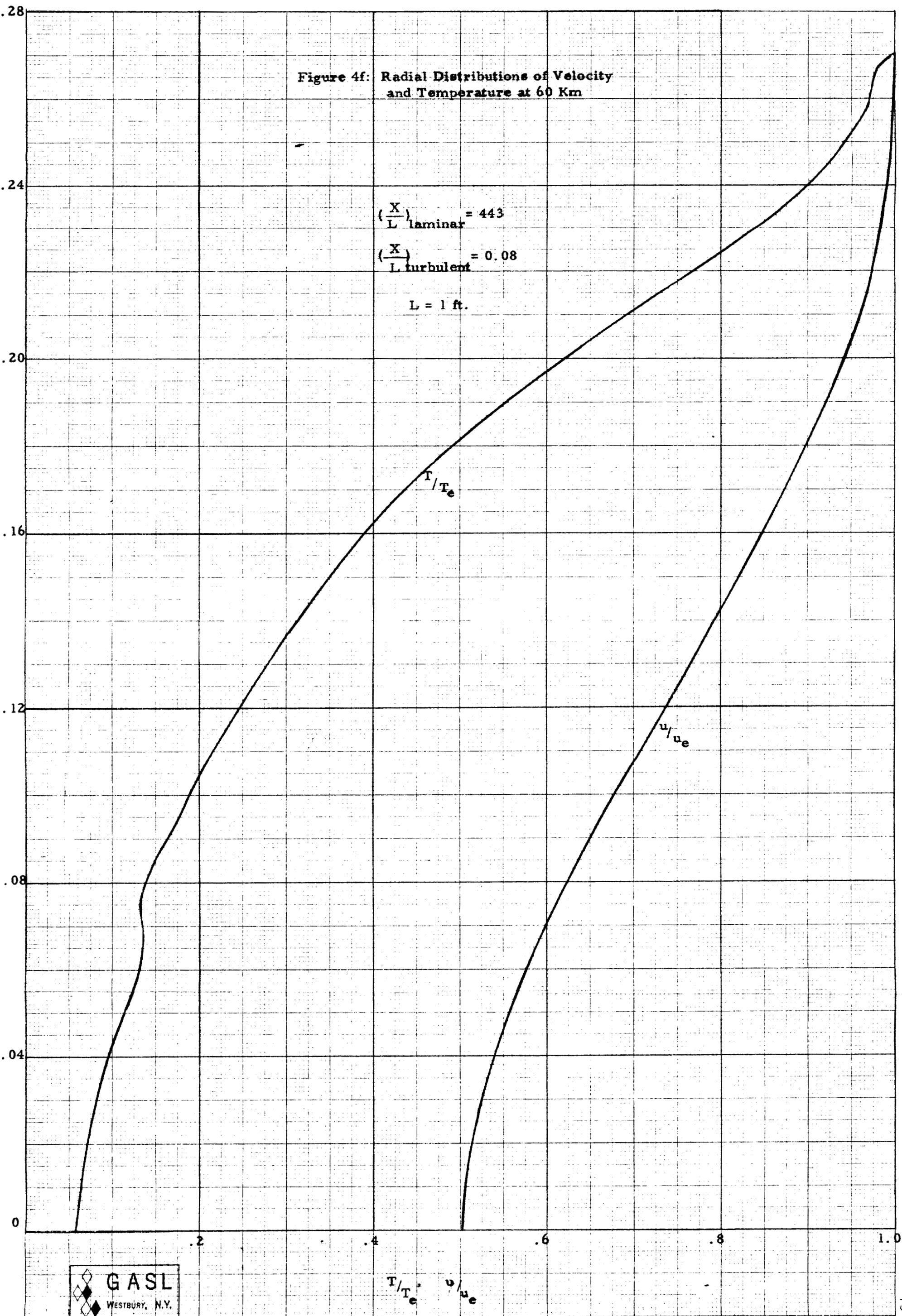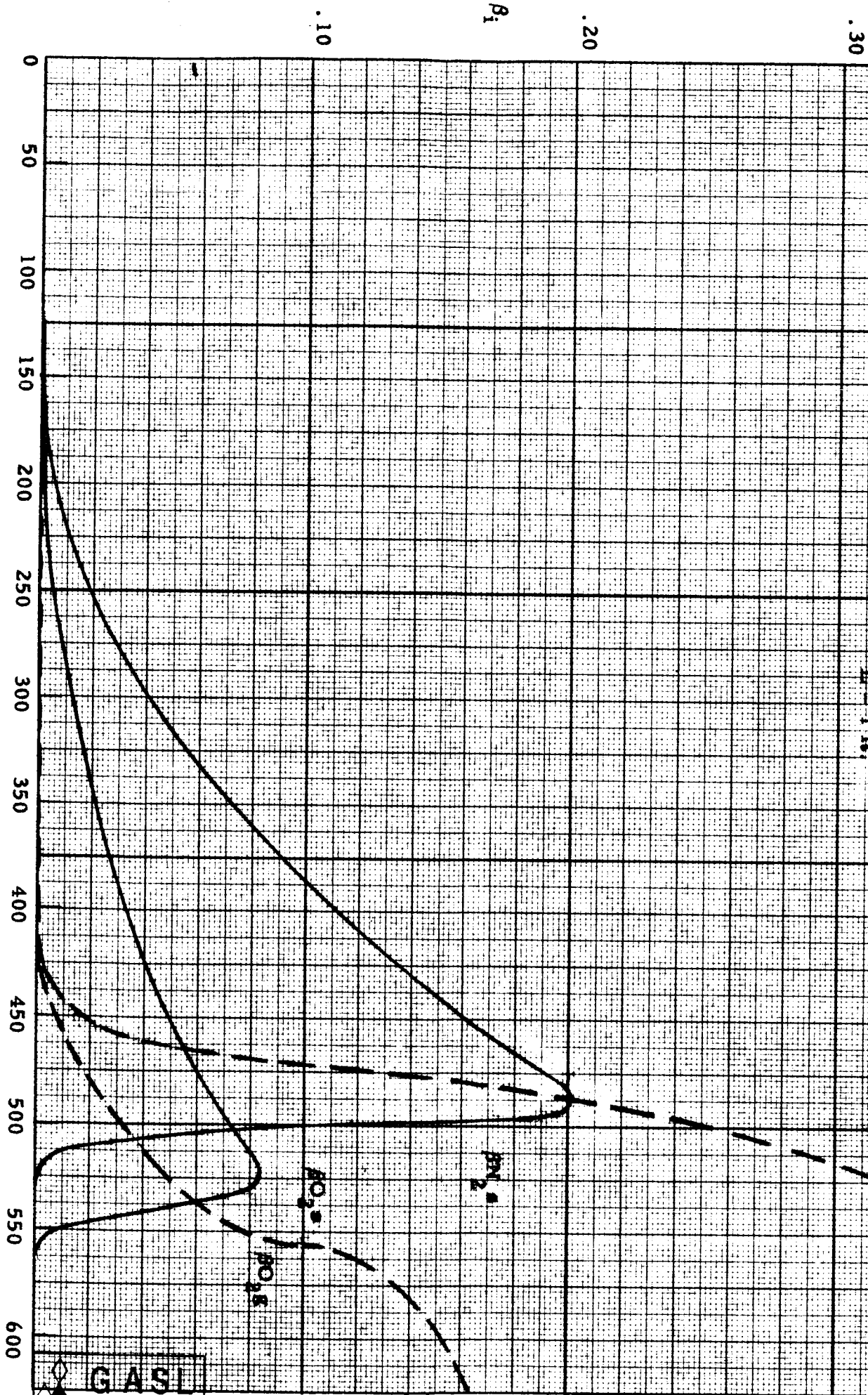Figure 4d. Radial Distributions of Velocity and Temperature at 60 Km

$$\left(\frac{X}{L}\right)_{laminar} = 123$$

$$\left(\frac{X}{L}\right)_{turbulent} = 0.17$$

$$L = 1 \text{ ft.}$$

$\frac{r}{L}$

T/T_e

u/u_e

T/T_e , u/u_e

GASL
WESTBURY, N.Y.

Figure 4e: Radial Distributions of Velocity and Temperature at 60 Km

$$\left(\frac{X}{L}\right)_{laminar} = 276$$

$$\left(\frac{X}{L}\right)_{turbulent} = 0.40$$

$$L = 1 \text{ ft.}$$

T/T_e

u/u_e

GASL
WESTBURY, N.Y.

u/u_e T/T_e

Figure 4f: **Radial Distributions of Velocity**
and Temperature at 60 Km

$$\left(\frac{X}{L}\right)_{laminar} = 443$$

$$\left(\frac{X}{L}\right)_{turbulent} = 0.08$$

$$L = 1 \text{ ft.}$$

T/T_e

u/u_e

.28

.24

.20

.16

.12

.08

.04

0

.2   .4   .6   .8   1.0

T/T_e u/u_e

GASL
WESTBURY, N.Y.

73

Figure 4g. Axial Distributions of Condensed Phase and Gas Phase Mass Fractions
Laminar Jet - 60 Km
$t_r = 1$ ft.

Figure 4h: Axial Distributions of Velocity and
Temperature - Turbulent Jet - 60 Km
L = 1 ft.

Figure 4h: Distributions of Velocity and Temperature

Axial

Laminar Jet, 60 Km

L = 1 ft.
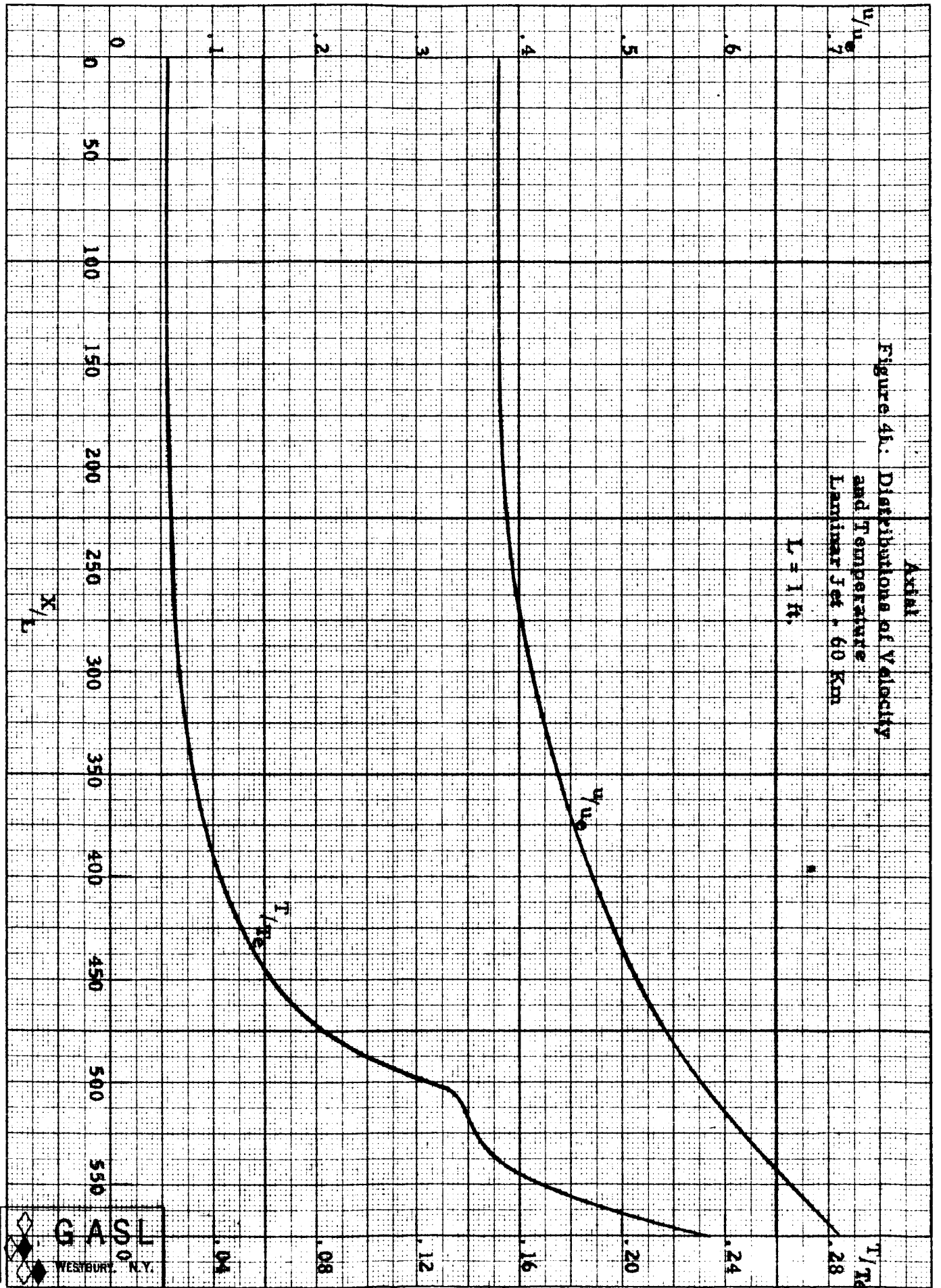
Figure 4j: Axial Distributions of Condensed Phase and Gas Phase Mass Fractions
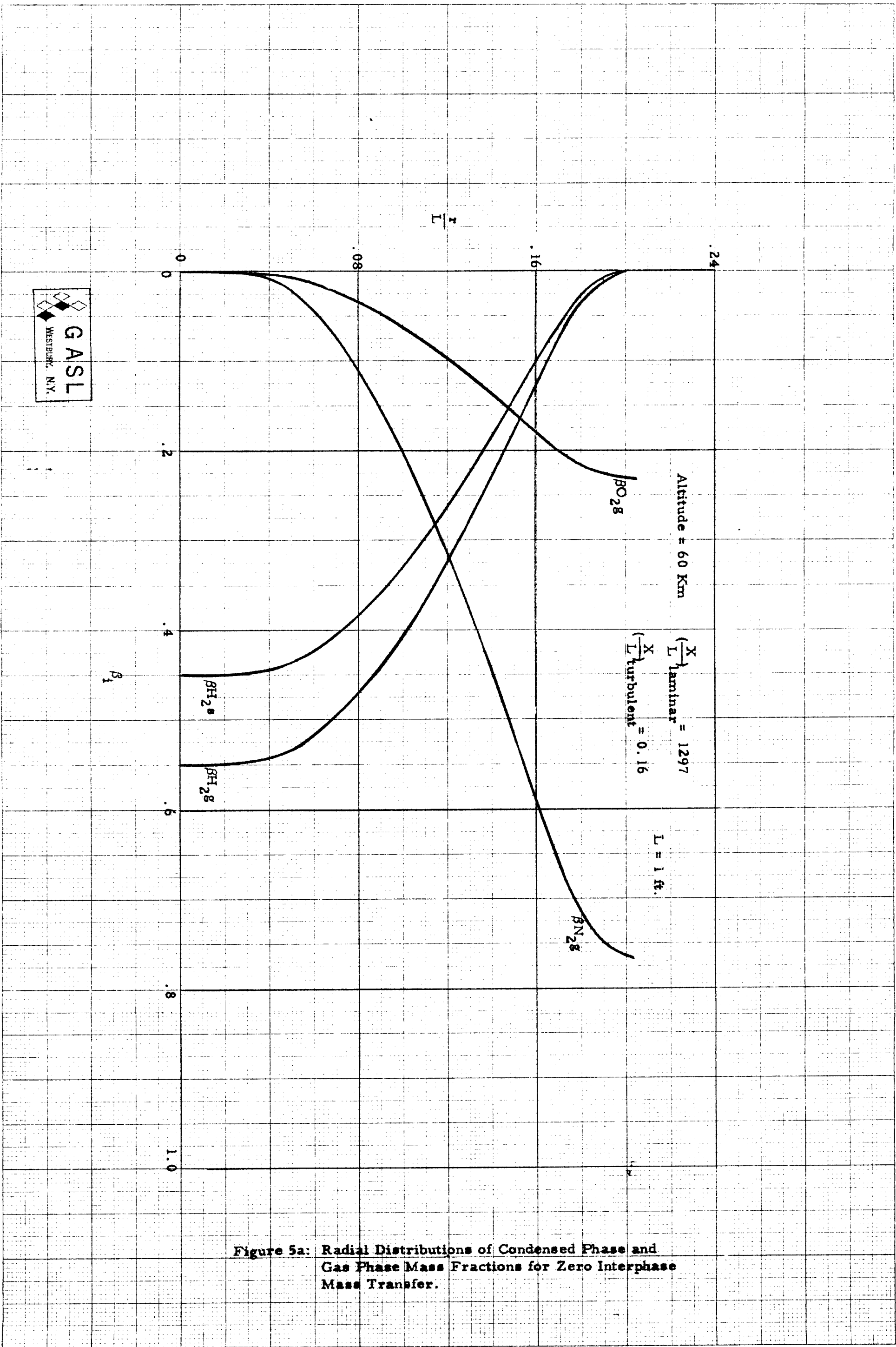Turbulent Jet - 60 Km
L = 1 ft
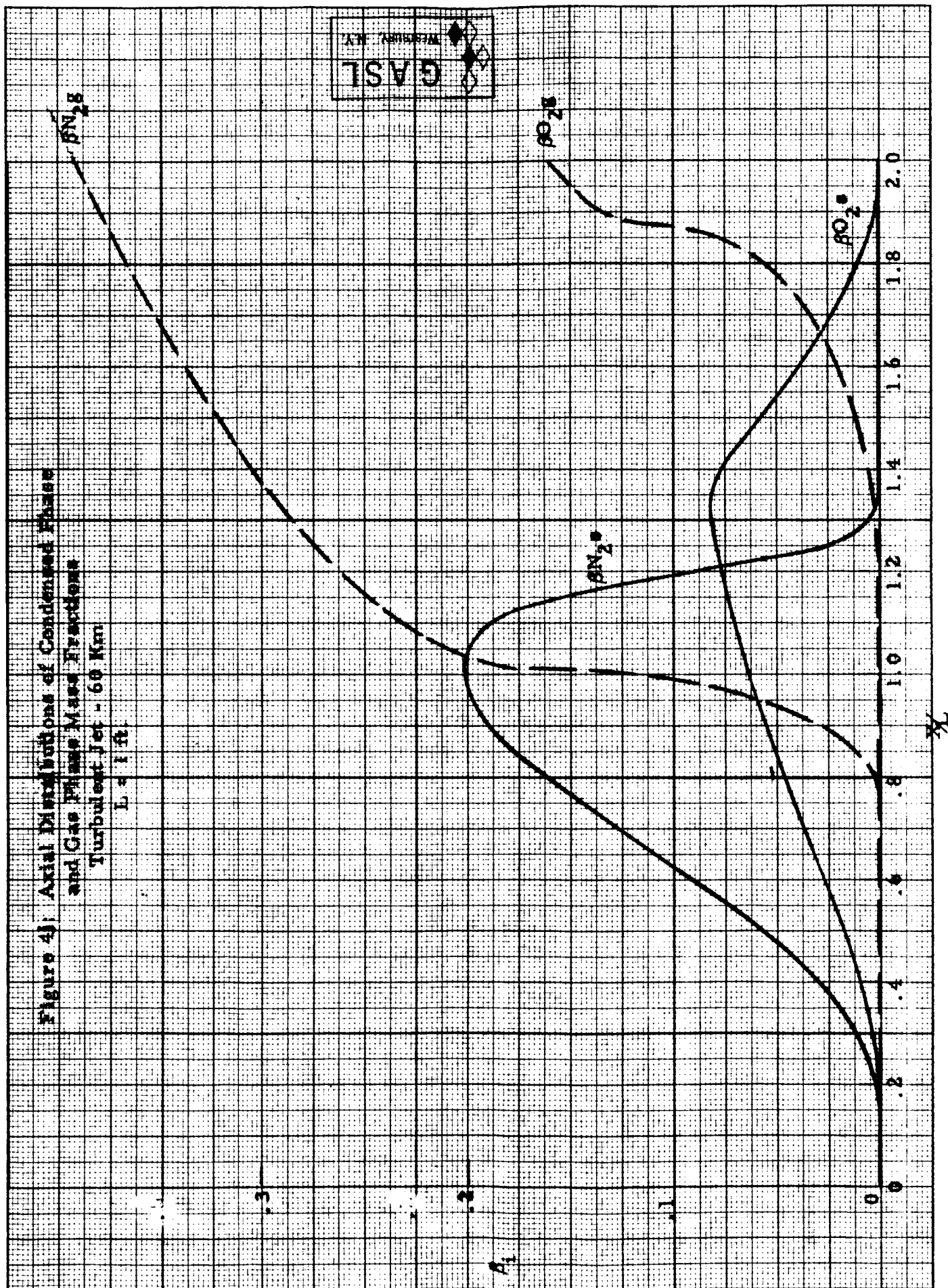
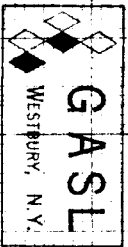Figure 5a: Radial Distributions of Condensed Phase and Gas Phase Mass Fractions for Zero Interphase Mass Transfer.

$\frac{r}{L}$

$\frac{\beta O_2 g}{}$

$\beta H_2 s$

$\beta H_2 g$

β_1

$\beta O_2 g$

Altitude = 60 Km

$\left(\frac{X}{L}\right)_{laminar} = 2930$

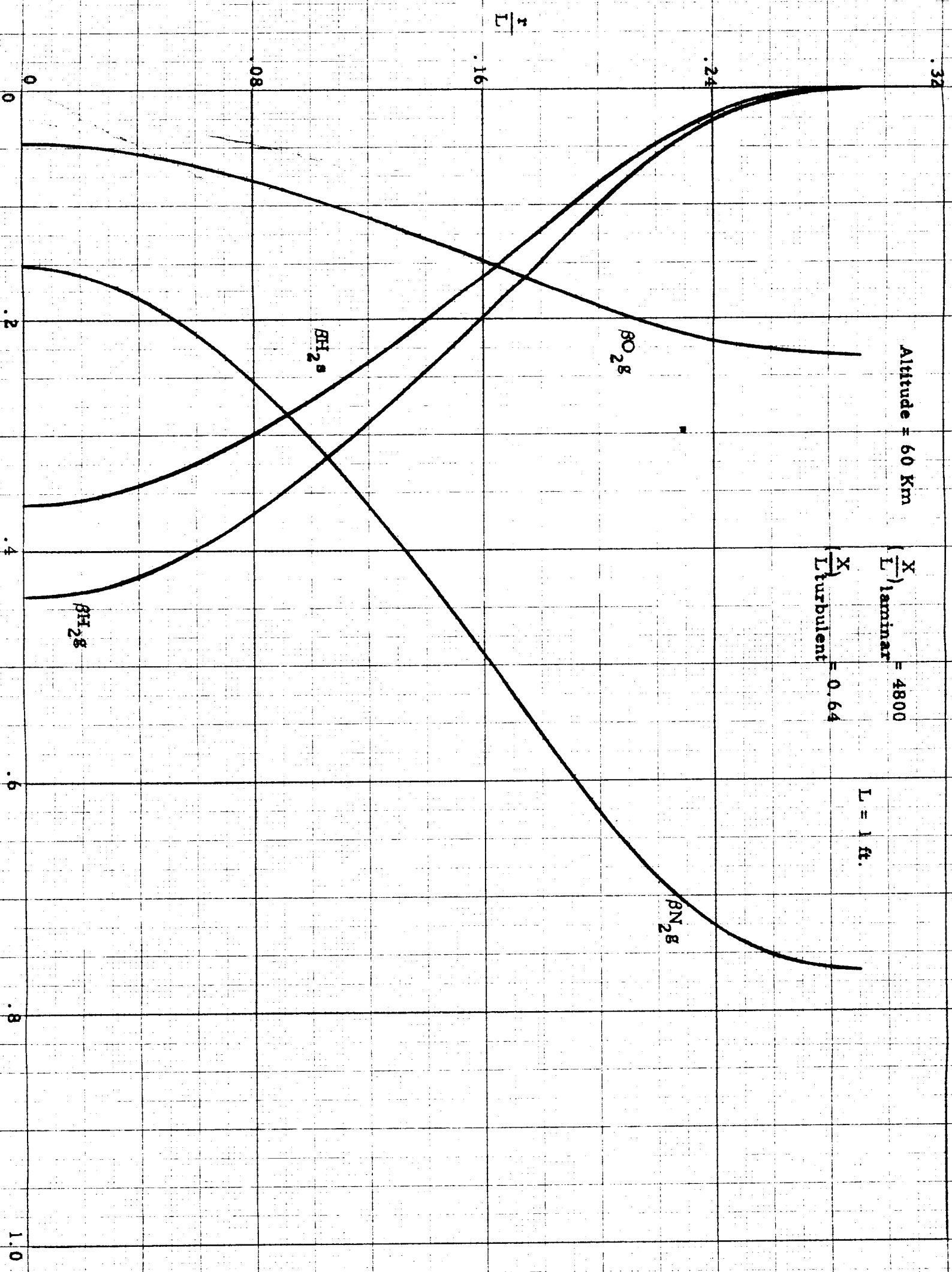$\left(\frac{X}{L}\right)_{turbulent} = 0.32$

L = 1 ft.
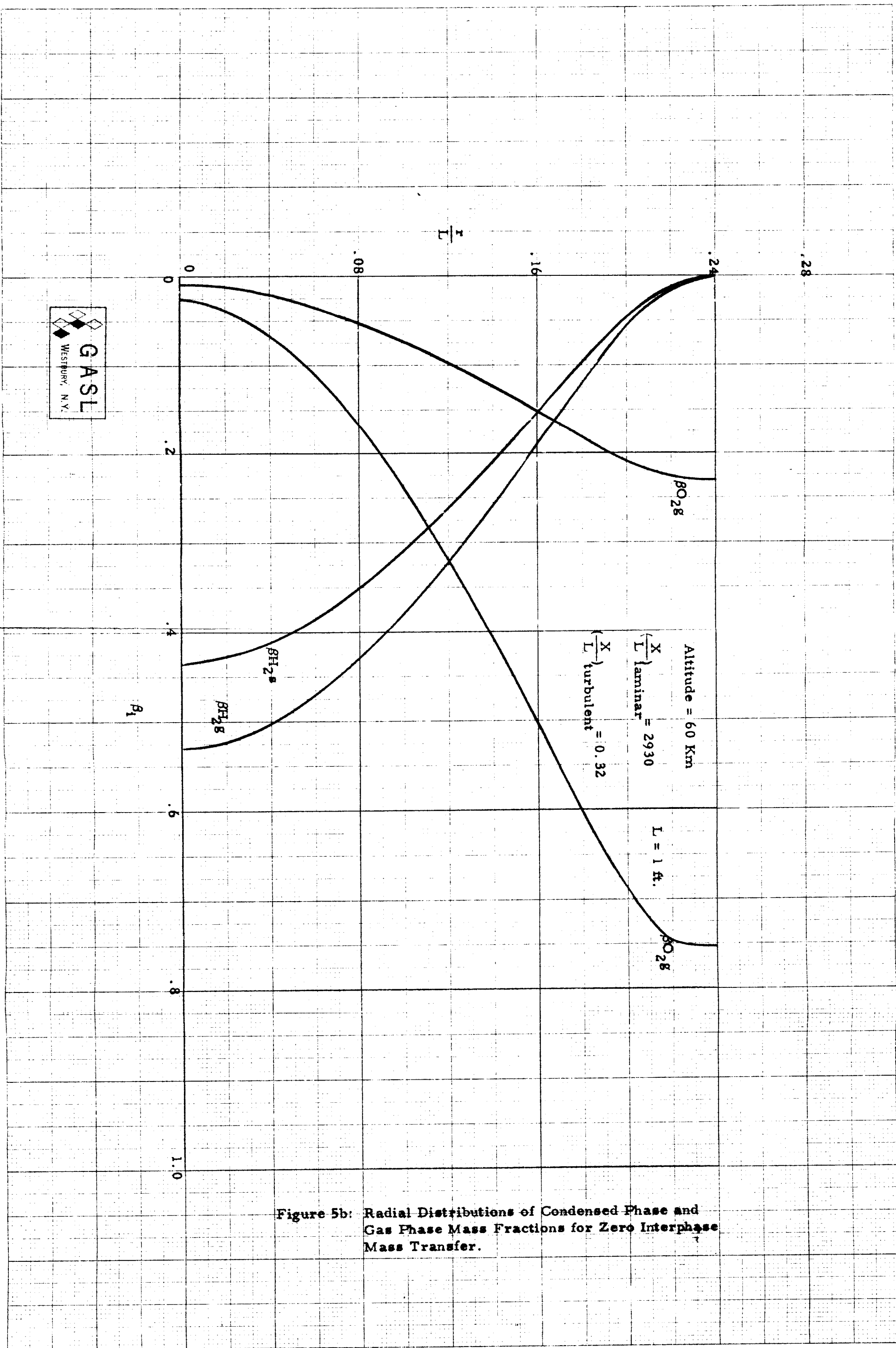
Figure 5b: Radial Distributions of Condensed Phase and
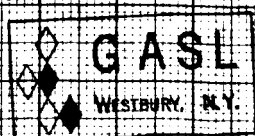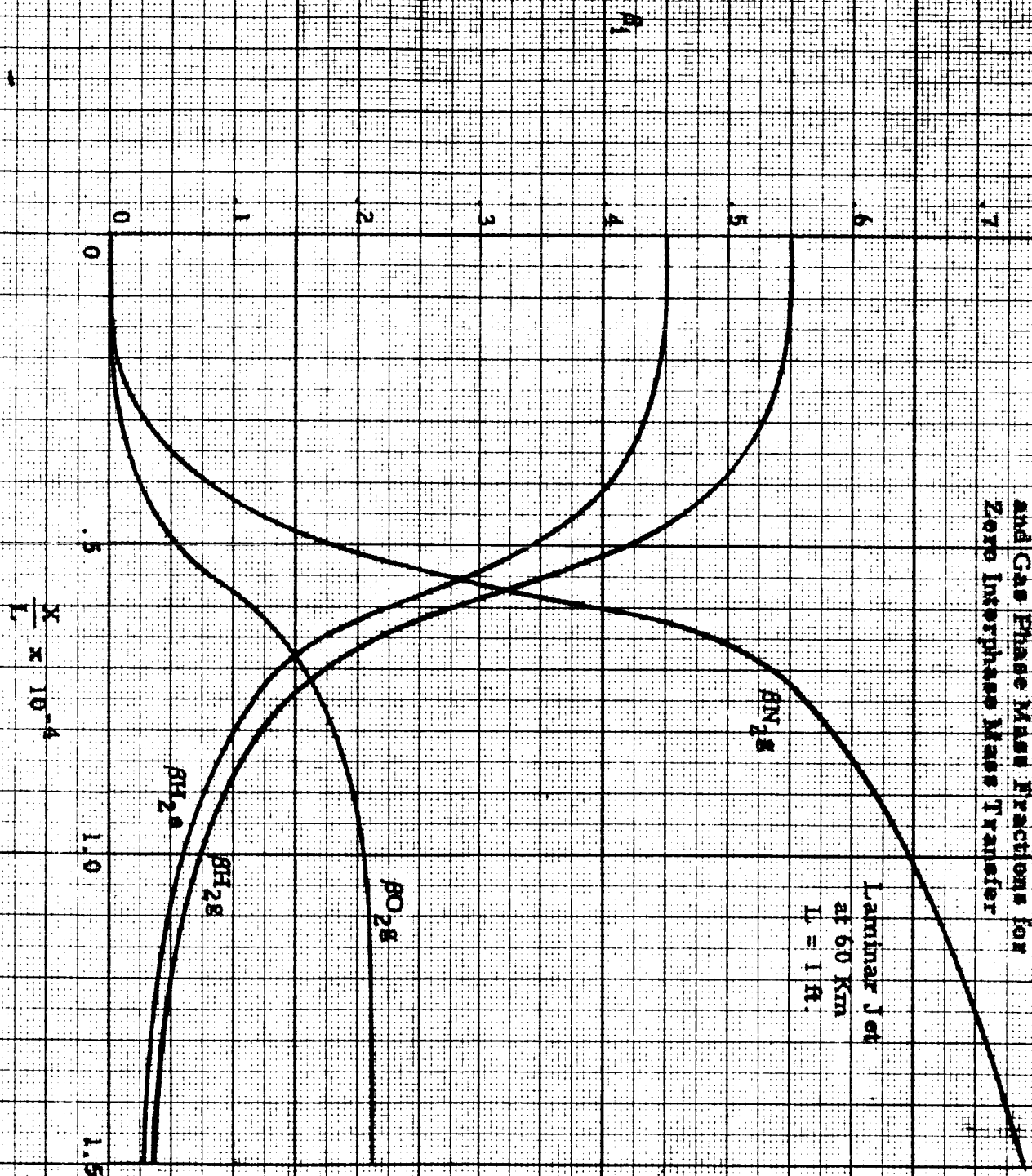Gas Phase Mass Fractions for Zero Interphase
Mass Transfer.

Figure 5c: Radial Distributions of Condensed Phase and
Gas Phase Mass Fractions for Zero Interphase
Mass Tranfser.

Figure 5d: Axial Distribution of Condensed Phase and Gas Phase Mass Fractions for Zero Interphase Mass Transfer

Laminar Jet at 60 Km L = 1 R.

Figure 5e: Axial Distributions of Velocity and Temperature
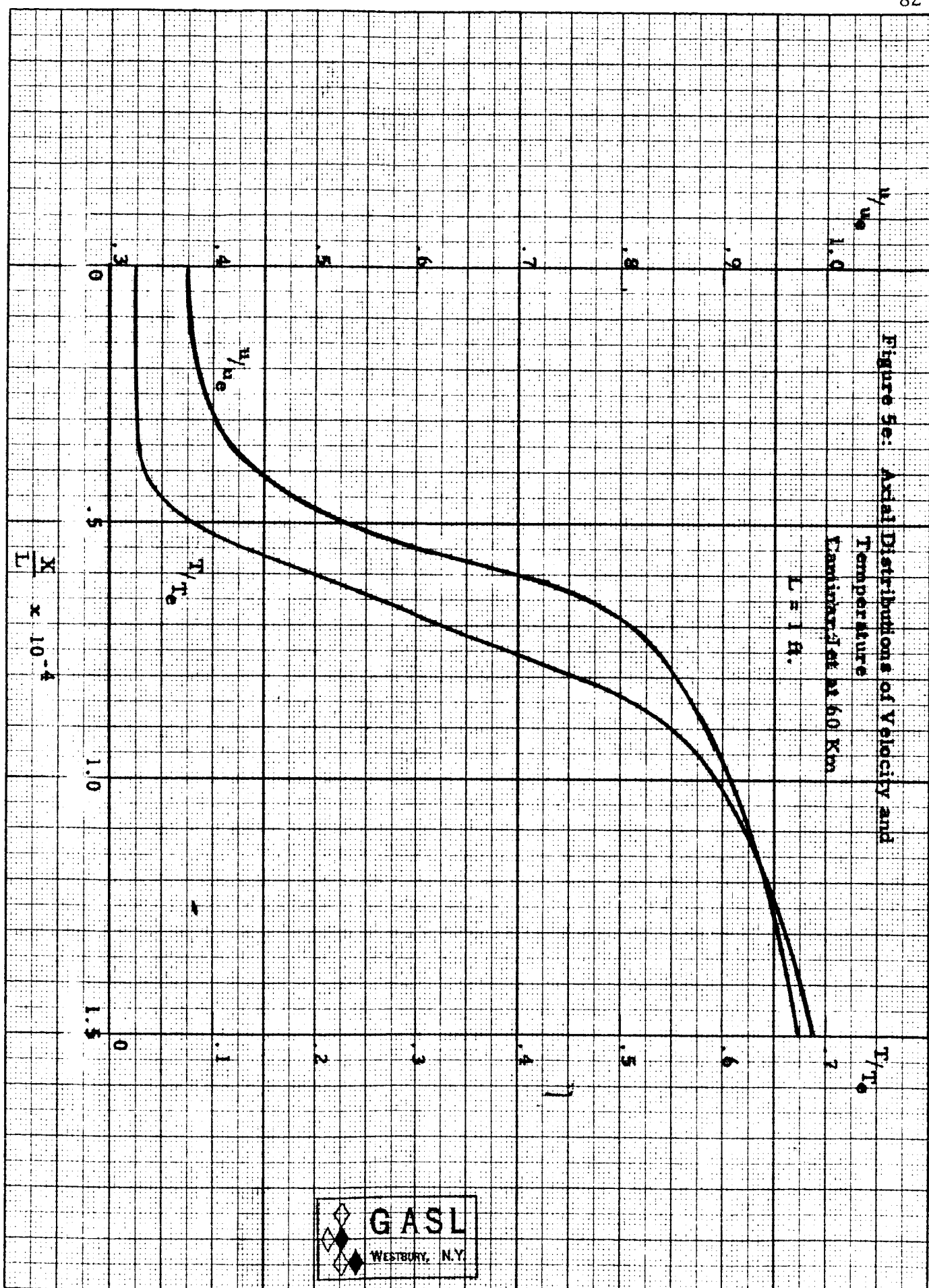
Combustor Jet at M 60 Km.

$L = 1$ ft.

Figure 51. Axial Distributions of Condensed Phase and Gas Phase Mass Fractions for Zero Interphase Mass Transfer

Figure 35: Axial Distributions of Velocity and Temperature

Turbulent Jet
at 60 Km
L = 1 ft.

GASL
Westbury, N.Y.